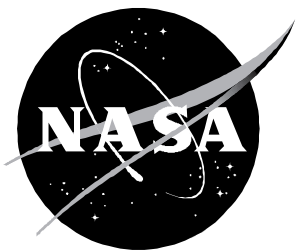


Computer Code for Determination of Thermally Perfect Gas Properties

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Summary

A set of compressible flow relations for a thermally perfect, calorically imperfect gas is derived for a value of c_p , expressed as a polynomial function of temperature, and developed into the thermally perfect gas (TPG) computer code. The code produces tables of compressible flow properties similar to those in NACA Rep. 1135. Unlike the tables of NACA Rep. 1135 that are valid only in the calorically perfect temperature regime, the TPG code results are also valid in the thermally perfect, calorically imperfect temperature regime, which considerably extends the range of temperature application. Accuracy of the TPG code in the calorically perfect temperature regime is verified by comparisons with the tables of NACA Rep. 1135. The small differences observed in this comparison result from inaccuracies of the tabulated values of NACA Rep. 1135, which originate from the calorically perfect gas assumption. In the thermally perfect, calorically imperfect temperature regime, the TPG code is validated by comparisons with results obtained with the method of NACA Rep. 1135 for calculating the thermally perfect, calorically imperfect compressible flow properties. The advantage of the TPG code is its applicability to any type of gas (monatomic, diatomic, triatomic, polyatomic, or any specified mixture thereof), whereas the method of NACA Rep. 1135 is restricted to only diatomic gases.

The temperature limits for application of the TPG code are also examined. The thermally perfect behavior of any gas species will terminate at some combination of low temperature and high pressure because of the presence of real gas effects and at some value of high temperature because of dissociation (except monatomic gases). Beyond these temperature limits, the TPG code may no longer accurately predict gas properties. However, within the temperature range in which the thermally perfect assumption is valid, the TPG code can accurately predict the compressible flow gas properties of any given gas species or mixture of species.

Introduction

The traditional computation of the one-dimensional (1-D) compressible flow gas properties is performed with one-dimensional calorically perfect gas equations such as those of NACA Rep. 1135. (See ref. 1.) If the gas of interest is air, then the tables of compressible flow values provided in NACA Rep. 1135 can be used. These tables were generated from the calorically perfect gas equations with a value of 1.40 for the ratio of specific heats γ . The application of these equations and tables is limited

to that range of temperature for which the calorically perfect gas assumption is valid. However, many aeronautical engineering calculations extend beyond the temperature limits of the calorically perfect gas assumption, and the application of the tables of NACA Rep. 1135 can result in significant errors. The temperature range limitation is greatly minimized by the assumption of a thermally perfect, calorically imperfect gas in the development of the compressible flow relations. (For simplicity, the term *thermally perfect* will be used throughout this paper to denote a thermally perfect, calorically imperfect gas.) This paper presents a computer code which implements one-dimensional compressible flow relations derived for a thermally perfect gas.

A calorically perfect gas is by definition a gas for which the values of specific heat at constant pressure c_p and specific heat at constant volume c_v are constants. Therefore, in the derivation of the compressible flow relations for a calorically perfect gas, the value of c_p was assumed constant. The calorically perfect gas equations are derived in many compressible flow textbooks and are summarized in NACA Rep. 1135. The accuracy of these equations is only as good as the assumption of a constant c_p (and therefore a constant γ). For any diatomic or polyatomic gas, the value of c_p actually varies with temperature and can only be approximated as a constant for a relatively narrow temperature range. At some point as the temperature increases, the c_p value begins to increase appreciably due to the excitation of the vibrational energy of the molecules. This phenomena occurs around 450 to 500 K for air. Thus, above 500 K, the use of $\gamma = 1.40$ for air in the calorically perfect gas equations will yield noticeably incorrect results. The variation of c_p with temperature (and only with temperature) continues up to approximately 1500 K. In this temperature range, where the value of c_p is only a function of temperature, air is considered a thermally perfect gas. Therefore, the derivation of the compressible flow relations for a thermally perfect gas must account for a variable heat capacity. Above 1500 K for air and at some relatively high temperature for all diatomic and polyatomic gases, dissociation of the molecules starts to occur. When dissociation commences, the value of c_p becomes a function of both temperature and pressure and the gas is no longer considered thermally perfect. The calorically perfect and thermally perfect temperature limits cited for air illustrate the much wider temperature range of application available from thermally perfect compressible flow relations.

The NACA Rep. 1135 presents one method for computation of the one-dimensional compressible

flow properties of a thermally perfect gas. In this approach, the variation of heat capacity due to the contribution from the vibrational energy mode of the molecule is determined from quantum mechanical considerations by the assumption of a simple harmonic vibrator model of a diatomic molecule. With this assumption, the vibrational contribution to the heat capacity of a diatomic gas takes the form of (ref. 2)

$$\left(\frac{c_p}{R}\right)_{\text{vib}} = \left(\frac{\Theta}{T}\right)^2 \frac{e^{\Theta/T}}{(e^{\Theta/T} - 1)^2} \quad (1)$$

where $\Theta = h\nu/k$, h is Planck's constant, ν is the characteristic frequency of molecular vibration, and k is the Boltzmann constant. The complete set of thermally perfect compressible flow relations based upon the c_p variation given in equation (1) is listed in NACA Rep. 1135 "Imperfect-Gas Effects." Tables of these thermally perfect gas properties are not provided because each value of total temperature T_t would yield a unique table of gas properties. The NACA Rep. 1135 does provide charts of the thermally perfect air properties normalized by the calorically perfect air values and plotted versus Mach number for select values of total temperature. This approach can only be applied to diatomic gases (e.g., N_2 , O_2 , and H_2) because of the functional form which describes the variation of heat capacity with temperature.

Because equation (1) is applicable to only diatomic gases, a different method for computing the one-dimensional compressible flow values of a thermally perfect gas was developed and is described in this paper. This method utilizes a polynomial curve fit of c_p versus temperature to describe the variation of heat capacity for a gas. The data required to generate this curve fit for a given gas can be found in tabulated form in several published sources such as the NBS "Tables of Thermal Properties of Gases" and the "JANAF Thermochemical Tables." (See refs. 3 and 4, respectively.) Actual coefficients for specific types of polynomial curve fits are also published in NASP TM-1107 and NASA SP-3001. (See refs. 5 and 6, respectively.) These curve fits, which are based upon tables of standard properties of gases, enable the application of this method to any type of gas; monotomic, diatomic, and polyatomic (e.g., H_2O , CO_2 , and CF_4) gases, or mixtures thereof are included, provided that known data sets of c_p versus temperature exist for the gases of interest.

A set of thermally perfect gas equations is derived for the specific heat as a polynomial function of

temperature and is presented in "Derivation of Thermally Perfect Gas Equations" in this report. This set of equations was then coded into a computer program referred to as the thermally perfect gas (TPG) code, which represents the end product of this research effort. The output tables of the TPG program are structured to resemble the tables of one-dimensional compressible flow properties that appear in NACA Rep. 1135; the difference between the two sets of tables is that the TPG code is valid in the thermally perfect temperature regime as well as in the calorically perfect temperature regime. This code serves the function of the tables of NACA Rep. 1135 for any gas species or mixture of gas species (e.g., air) and significantly increases the range of valid temperature application.

Symbols

a	speed of sound
A	cross-sectional area of stream tube or channel
A_j	coefficients of polynomial curve fit for $\frac{c_p}{R}$
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
e	internal energy per unit mass
h	enthalpy per unit mass, $e + pv$; Planck's constant
k	Boltzmann constant
M	Mach number, $\frac{V}{a}$
p	static pressure
q	dynamic pressure, $\frac{\rho V^2}{2}$; heat added per unit mass
R	specific gas constant
\mathcal{R}	universal gas constant
s	entropy per unit mass
T	static temperature
u	velocity component parallel to free-stream flow direction
v	specific volume, $\frac{1}{\rho}$
V	speed of flow
w	external work performed per unit mass
W	molecular weight

X	mole fraction	jmax	maximum j value
Y	mass fraction	lim	temperature limit (upper or lower) of polynomial curve fit for c_p
Z	compressibility factor	mix	gas mixture
β	$\sqrt{ M^2 - 1 }$	n	total number of gas species that comprise gas mixture
δ	increment indicator	rev	reversible
γ	ratio of specific heats, $\frac{c_p}{c_v}$	perf	quantity evaluated for gas that is both thermally and calorically perfect
Θ	constant of molecular vibrational energy	therm perf	quantity evaluated for gas that is thermally perfect but calorically imperfect
ν	characteristic frequency of molecu- lar vibration	vib	vibrational contribution
ρ	static mass density		
Subscripts:		Abbreviations:	
1	conditions just upstream of shock wave	1-D	one-dimensional
2	conditions just downstream of shock wave	JANAF	Joint Army-Navy-Air Force
t	total (stagnation) conditions	NACA	National Advisory Committee for Aeronautics
*	critical (sonic) conditions	NASP	National Aero-Space Plane
i	i th component gas species of mixture	NBS	National Bureau of Standards
j	j th coefficient of polynomial curve fit for c_p	TPG	thermally perfect gas

Derivation of Thermally Perfect Gas Equations

Polynomial Curve Fit for c_p

The selection of a suitable curve fit function for c_p is the starting point for the development of thermally perfect compressible flow relations. The form chosen for the TPG code was the eight-term, fifth-order polynomial expression given below in which the value of c_p has been nondimensionalized by the species gas constant.

$$\frac{c_p}{R} = A_1 \left(\frac{1}{T^2} \right) + A_2 \left(\frac{1}{T} \right) + A_3 + A_4(T) + A_5(T^2) + A_6(T^3) + A_7(T^4) + A_8(T^5) = \sum_{j=1}^8 A_j T^{j-3} \quad (2)$$

For a given temperature range, A_1 to A_8 are the coefficients of the curve fit. This is the functional form for c_p of reference 5, which provides values of A_1 to A_8 for 15 different gas species. Reference 6 provides similar c_p/R coefficient data for over 200 different gas species for a five-term, fourth-order polynomial curve fit equation (A_3 to A_7). Equation (2) is also valid with these coefficients provided that A_1 , A_2 , and A_8 are set equal to zero. If the pertinent c_p/R versus temperature data fits some other algebraic expression, then that expression could easily be substituted for equation (2) in the TPG code. This issue will be addressed further in "TPG Code Description." The only requirement is that closed-form solutions to both $\int c_p dT$ and $\int \frac{c_p}{T} dT$ must be known; the reason will become apparent as the gas expansion relations are derived for a thermally perfect gas.

The TPG code can compute the thermally perfect gas properties for not only individual gas species but also for mixtures of individual gas species (e.g., air). This code capability is achieved by calculating the variation of the heat capacity for the specified gas mixture. The c_p of a mixture of gases is computed from

$$c_{p,\text{mix}} = \sum_{i=1}^n Y_i c_{p,i} \quad (3)$$

where Y_i is the mass fraction of the i th gas species. The value of $c_{p,i}$ is determined from equation (2) for each component species. The following example of standard air, consisting of the four major component gas species N_2 , O_2 , Ar , and CO_2 , illustrates how this equation is actually implemented in the code.

$$c_{p,\text{air}} = Y_{\text{N}_2} c_{p,\text{N}_2} + Y_{\text{O}_2} c_{p,\text{O}_2} + Y_{\text{Ar}} c_{p,\text{Ar}} + Y_{\text{CO}_2} c_{p,\text{CO}_2} \quad (4)$$

Equation (4) can be fully expanded with the use of equation (2) to give

$$\begin{aligned} c_{p,\text{air}} = & Y_{\text{N}_2} R_{\text{N}_2} A_{1,\text{N}_2} \left(\frac{1}{T^2} \right) + Y_{\text{N}_2} R_{\text{N}_2} A_{2,\text{N}_2} \left(\frac{1}{T} \right) + \cdots + Y_{\text{N}_2} R_{\text{N}_2} A_{8,\text{N}_2} T^5 \\ & + Y_{\text{O}_2} R_{\text{O}_2} A_{1,\text{O}_2} \left(\frac{1}{T^2} \right) + Y_{\text{O}_2} R_{\text{O}_2} A_{2,\text{O}_2} \left(\frac{1}{T} \right) + \cdots + Y_{\text{O}_2} R_{\text{O}_2} A_{8,\text{O}_2} T^5 \\ & + Y_{\text{Ar}} R_{\text{Ar}} A_{1,\text{Ar}} \left(\frac{1}{T^2} \right) + Y_{\text{Ar}} R_{\text{Ar}} A_{2,\text{Ar}} \left(\frac{1}{T} \right) + \cdots + Y_{\text{Ar}} R_{\text{Ar}} A_{8,\text{Ar}} T^5 \\ & + Y_{\text{CO}_2} R_{\text{CO}_2} A_{1,\text{CO}_2} \left(\frac{1}{T^2} \right) + Y_{\text{CO}_2} R_{\text{CO}_2} A_{2,\text{CO}_2} \left(\frac{1}{T} \right) + \cdots + Y_{\text{CO}_2} R_{\text{CO}_2} A_{8,\text{CO}_2} T^5 \end{aligned} \quad (5)$$

By combining like terms in equation (5), a resultant c_p curve for the gas mixture (air) is generated.

$$c_{p,\text{air}} = A_{1,\text{air}} \left(\frac{1}{T^2} \right) + A_{2,\text{air}} \left(\frac{1}{T} \right) + A_{3,\text{air}} + A_{4,\text{air}} T + A_{5,\text{air}} T^2 + A_{6,\text{air}} T^3 + A_{7,\text{air}} T^4 + A_{8,\text{air}} T^5 \quad (6a)$$

where

$$A_{j,\text{air}} = Y_{\text{N}_2} R_{\text{N}_2} A_{j,\text{N}_2} + Y_{\text{O}_2} R_{\text{O}_2} A_{j,\text{O}_2} + Y_{\text{Ar}} R_{\text{Ar}} A_{j,\text{Ar}} + Y_{\text{CO}_2} R_{\text{CO}_2} A_{j,\text{CO}_2} \quad (j = 1 \text{ to } 8) \quad (6b)$$

In generalized terminology, equations (6a) and (6b) are expressed as

$$c_{p,\text{mix}} = \sum_{j=1}^{\text{jmax}} A_{j,\text{mix}} T^{j-3} \quad (7a)$$

and

$$A_{j,\text{mix}} = \sum_{i=1}^n Y_i R_i A_{j,i} \quad (j = 1, \dots, \text{jmax}) \quad (7b)$$

Gas Expansion Relations

Parameter γ . With a known curve fit expression for c_p of the gas mixture, the value of γ for a given temperature can be computed directly from its definition and the thermally perfect relation between c_p and c_v .

$$c_p - c_v = R \quad (8)$$

and

$$\gamma \equiv \frac{c_p}{c_v} = \frac{c_p}{c_p - R} \quad (9)$$

The gas constant R for the mixture is calculated by dividing the universal gas constant \mathcal{R} by the molecular weight of the mixture W_{mix} ,

$$R = \frac{\mathcal{R}}{W_{\text{mix}}} \quad (10)$$

where

$$W_{\text{mix}} = \sum_{i=1}^n X_i W_i \quad (11)$$

X_i is the mole fraction of each component species determined from

$$X_i = \frac{Y_i}{W_i \sum_{k=1}^n \frac{Y_k}{W_k}} \quad (12)$$

Parameters u , a , M , and T/T_t . If the flow is assumed to be adiabatic, then the 1-D energy equation written for two separate points in the flow field is (ref. 7)

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \quad (13)$$

where the enthalpy h referenced to 0 K is given by

$$h = \int_0^T c_p dT \quad (14)$$

Therefore,

$$\int_0^{T_1} c_p dT + \frac{u_1^2}{2} = \int_0^{T_2} c_p dT + \frac{u_2^2}{2} \quad (15)$$

If point 2 is selected to represent the stagnation condition, then $u_2 = 0$ and $T_2 = T_t$. Then equation (15) reduces to

$$\int_0^{T_1} c_p dT + \frac{u_1^2}{2} = \int_0^{T_t} c_p dT \quad (16)$$

or

$$\frac{u_1^2}{2} = \int_0^{T_t} c_p dT - \int_0^{T_1} c_p dT = \int_{T_1}^{T_t} c_p dT \quad (17)$$

where for the selected fifth-order curve fit for c_p (eqs. (7a) and (7b) with jmax = 8)

$$\begin{aligned} \int_{T_1}^{T_t} c_p dT = & -A_1 \left(\frac{1}{T_t} - \frac{1}{T_1} \right) + A_2 \ln \frac{T_t}{T_1} + A_3 (T_t - T_1) + \frac{A_4}{2} (T_t^2 - T_1^2) + \frac{A_5}{3} (T_t^3 - T_1^3) \\ & + \frac{A_6}{4} (T_t^4 - T_1^4) + \frac{A_7}{5} (T_t^5 - T_1^5) + \frac{A_8}{6} (T_t^6 - T_1^6) \end{aligned} \quad (18)$$

For a specified total temperature, the value of equation (18) can be computed for a range of static temperatures. Each value of static temperature T_1 (T_1 less than T_t) represents a unique point in the expansion of the gas from its stagnation conditions. In the temperature increment mode of the TPG program, the user selects the total temperature, the desired static temperature increment, and the upper and lower limits for the static temperature range. The program simply increments downward through the selected static temperature range and computes all of the compressible flow properties for each value of static temperature. The value of T_1/T_t is therefore not actually computed from any equation but rather is a result of this incremental procedure. From equation (17), the expression for the velocity becomes

$$u_1 = \sqrt{2 \int_{T_1}^{T_t} c_p dT} \quad (19)$$

The speed of sound for a thermally perfect gas is given by

$$a_1 = \sqrt{\gamma_1 R T_1} \quad (20)$$

and from the definition of Mach number

$$M_1 = \frac{u_1}{a_1} \quad (21)$$

Parameter p/p_t . The first law of thermodynamics

$$\delta q + \delta w = de \quad (22)$$

and the definition of entropy

$$\delta q_{\text{rev}} = T ds \quad (23)$$

along with the thermodynamic relation

$$\delta w = -p dv \quad (24)$$

yield

$$T ds = de + p dv \quad (25)$$

From the definition of enthalpy,

$$h = e + pv \quad (26)$$

differentiation gives

$$dh = de + p dv + v dp \quad (27)$$

The combination of equations (25) and (27) produces

$$T ds = dh - v dp \quad (28)$$

For a thermally perfect gas,

$$dh = c_p dT \quad (29)$$

The substitution of equation (29) into equation (28) and the definition of specific volume result in

$$ds = c_p \frac{dT}{T} - \frac{dp}{\rho T} \quad (30)$$

Substitution of the equation of state $p = \rho RT$, which is valid for a thermally perfect gas, gives

$$ds = c_p \frac{dT}{T} - R \frac{dp}{p} \quad (31)$$

Integration of equation (31) between two different thermodynamic states yields

$$s_2 - s_1 = \int_{T_1}^{T_2} \frac{c_p}{T} dT - R \left(\ln \frac{p_2}{p_1} \right) \quad (32)$$

For an isentropic path from state 1 to state 2, $s_2 - s_1 = 0$ and therefore

$$R \left(\ln \frac{p_2}{p_1} \right) = \int_{T_1}^{T_2} \frac{c_p}{T} dT \quad (33)$$

If state 2 represents the stagnation condition, then equation (33) can be rewritten as

$$\frac{p_1}{p_t} = \frac{1}{\exp \left(\frac{1}{R} \int_{T_1}^{T_t} \frac{c_p}{T} dT \right)} \quad (34)$$

and for the selected fifth-order curve fit for c_p , the closed-form solution to the integral in equation (34) is

$$\begin{aligned} \int_{T_1}^{T_t} \frac{c_p}{T} dT = & -\frac{A_1}{2} \left(\frac{1}{T_t^2} - \frac{1}{T_1^2} \right) - A_2 \left(\frac{1}{T_t} - \frac{1}{T_1} \right) + A_3 \ln \frac{T_t}{T_1} + A_4 (T_t - T_1) + \frac{A_5}{2} (T_t^2 - T_1^2) \\ & + \frac{A_6}{3} (T_t^3 - T_1^3) + \frac{A_7}{4} (T_t^4 - T_1^4) + \frac{A_8}{5} (T_t^5 - T_1^5) \end{aligned} \quad (35)$$

Equations (34) and (35) are used in the TPG code to compute the value of p_1/p_t for each value of T_1 .

Parameter q/p_t . A relation for the ratio of dynamic to total pressure q/p_t for a given T_1 results from the following expression

$$\frac{q_1}{p_t} = \frac{q_1}{p_1} \left(\frac{p_1}{p_t} \right) \quad (36)$$

Then q_1/p_1 for a thermally perfect gas can be expressed with the use of the equation of state, the definition of Mach number, and the equation for the speed of sound as

$$\frac{q_1}{p_1} = \frac{\frac{1}{2} \rho_1 V_1^2}{p_1} = \frac{\frac{1}{2} V_1^2}{RT_1} = \frac{\frac{1}{2} \left(\frac{V_1^2}{a_1^2} \right)}{\frac{RT_1}{a_1^2}} = \frac{\frac{1}{2} M_1^2}{\frac{RT_1}{\gamma_1 RT_1}} = \frac{\gamma_1}{2} M_1^2 \quad (37)$$

Parameters ρ/ρ_t and A/A_* . With the knowledge of p/p_t and T/T_t , the value of ρ/ρ_t can be determined from the equation of state

$$p_1 = \rho_1 RT_1 \quad (38)$$

and

$$p_t = \rho_t RT_t \quad (39)$$

Equation (38) is divided by equation (39) to give

$$\frac{\rho_1}{\rho_t} = \left(\frac{p_1}{p_t} \right) \left(\frac{T_t}{T_1} \right) \quad (40)$$

Now the value of A_1/A_* is obtained by the use of the 1-D continuity equation.

$$\rho_1 u_1 A_1 = \rho_* u_* A_* \quad (41)$$

Equation (41) can be rewritten as

$$\rho_{t,1} \left(\frac{\rho_1}{\rho_{t,1}} \right) u_1 A_1 = \rho_{t,*} \left(\frac{\rho_*}{\rho_{t,*}} \right) u_* A_* \quad (42)$$

For isentropic flow, the value of ρ_t is constant ($\rho_{t,1} = \rho_{t,*}$) and thus equation (42) becomes

$$\left(\frac{\rho_1}{\rho_t} \right) u_1 A_1 = \left(\frac{\rho_*}{\rho_t} \right) u_* A_* \quad (43)$$

The solution for A_1/A_* gives

$$\frac{A_1}{A_*} = \frac{\left(\frac{\rho_*}{\rho_t} \right) u_*}{\left(\frac{\rho_1}{\rho_t} \right) u_1} \quad (44)$$

As equation (44) indicates, before the value of A_1/A_* can be computed for any given value of T_1 , the values of ρ_*/ρ_t and u_* must be known. The TPG code is written to calculate all of the compressible flow properties at

the sonic point temperature T_* before the calculation of these properties at any other T_1 values. The value of T_* is obtained from equations (19), (20), and (21) for the condition $M_1 = 1$ ($u_1 = a_1$). This gives

$$2 \int_{T_*}^{T_i} c_p dT = \gamma_* R T_* \quad (45)$$

and equation (9) then yields

$$2 \int_{T_*}^{T_i} c_p dT = \left(\frac{c_p}{c_p - R} \right) R T_* \quad (46)$$

Equation (46) can be expressed in terms of only one unknown T_* by the use of equations (7a) and (18). An iterative technique is implemented in the TPG code to solve for T_* in equation (46).

Normal Shock Relations

Parameters T_2 , γ_2 , u_2 , a_2 , and M_2 . The continuity and momentum equations for 1-D flow across a normal shock wave are given in equations (47) and (48), respectively.

$$\rho_1 u_1 = \rho_2 u_2 \quad (47)$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \quad (48)$$

The momentum equation is divided by the continuity equation to give

$$\frac{p_1}{\rho_1 u_1} + u_1 = \frac{p_2}{\rho_2 u_2} + u_2 \quad (49)$$

The relation for the speed of sound, equation (20), can be written with the use of the equation of state as

$$a^2 = \frac{\gamma p}{\rho} \quad (50)$$

The solution of equation (50) for p and substitution into equation (49) yield

$$\frac{a_1^2}{\gamma_1 u_1} + u_1 = \frac{a_2^2}{\gamma_2 u_2} + u_2 \quad (51)$$

Equation (51) provides the needed relationship across the shock wave. For a given value of T_1 , the left-hand side of equation (51) is obtained from equations (9), (19), and (20). The right-hand side of equation (51) apparently has three unknowns γ_2 , u_2 , and a_2 , but in reality these three variables are all functions of only T_2 . (Actually, u_2 depends on both T_2 and $T_{t,2}$, but because a shock wave is considered adiabatic, $h_{t,2} = h_{t,1}$; this translates to $T_{t,2} = T_{t,1}$ for a thermally perfect gas because c_p is a function of temperature only.) Therefore, from equations (7a), (9), (18), (19), and (20), the right-hand side of equation (51) can be expressed as a single elementary, nonlinear function of T_2 . An iterative technique has been implemented in the TPG code to solve equation (51) for T_2 . With the known value of T_2 , equations (9), (19), (20), and (21) determine the values of γ_2 , u_2 , a_2 , and M_2 , respectively. The desired shock relations, T_2/T_1 and u_2/u_1 , can then be computed.

Parameters p_2/p_1 and ρ_2/ρ_1 . The 1-D momentum equation in the form

$$p_2 - p_1 = \rho_1 u_1^2 - \rho_2 u_2^2 \quad (52)$$

and the continuity equation expressed as

$$\rho_2 = \frac{\rho_1 u_1}{u_2} \quad (53)$$

give

$$p_2 - p_1 = \rho_1 u_1 (u_1 - u_2) = \rho_1 u_1^2 \left(1 - \frac{u_2}{u_1} \right) \quad (54)$$

Equation (54) is divided by p_1 , and from equation (50) ρ_1/p_1 is expressed as $\gamma_1/(a_1)^2$ which gives

$$\frac{p_2 - p_1}{p_1} = \gamma_1 M_1^2 \left(1 - \frac{u_2}{u_1}\right) \quad (55)$$

The expression for p_2/p_1 is then

$$\frac{p_2}{p_1} = 1 + \gamma_1 M_1^2 \left(1 - \frac{u_2}{u_1}\right) \quad (56)$$

where the values of γ_1 and M_1 are obtained from equations (9) and (21), respectively, and the value for u_2/u_1 is obtained from equation (51) as discussed in the previous section. With a known value of u_2/u_1 , the value of ρ_2/ρ_1 is determined directly from the continuity equation.

$$\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \quad (57)$$

Parameters $p_{t,2}/p_{t,1}$ and $p_1/p_{t,2}$. The value of the total pressure loss $p_{t,2}/p_{t,1}$ can now be computed from a combination of static and total pressure ratios.

$$\frac{p_{t,2}}{p_{t,1}} = \frac{\left(\frac{p_{t,2}}{p_2}\right)}{\left(\frac{p_{t,1}}{p_1}\right)} \left(\frac{p_2}{p_1}\right) \quad (58)$$

The values of $p_{t,1}/p_1$ and $p_{t,2}/p_2$ are determined from equation (34) evaluated at T_1 and T_2 , respectively, while p_2/p_1 is obtained from equation (56). Similarly, the pitot-static tube pressure ratio $p_1/p_{t,2}$ is calculated from

$$\frac{p_1}{p_{t,2}} = \left(\frac{p_{t,1}}{p_{t,2}}\right) \left(\frac{p_1}{p_{t,1}}\right) \quad (59)$$

TPG Code Description

An interactive computer code, herein referred to as the TPG code, has been written based on the equations described previously. This code delivers a complete table of results within seconds when run on a minimally configured workstation. The purpose of the code is the output of tables of compressible flow properties for a thermally perfect gas or mixture of gases styled after the tables of NACA Rep. 1135. Output may be in the form of a single table of gas expansion properties, a single table of gas expansion properties and normal shock properties, or separate tables of gas expansion and normal shock properties. The entries within the tables are based upon constant decrements of static temperature or constant increments of Mach number. Such entries in terms of static temperature decrements reveal a fundamental difference between the data of the TPG code and NACA Rep. 1135. This fundamental difference is highlighted when the TPG code output tables, displayed as constant decrements of static temperature, are compared with the calorically perfect gas table of NACA Rep. 1135, a single table of compressible

flow properties for air as a function of Mach number. The properties of thermally perfect gases vary with both total temperature T_t and local static temperature T rather than with only the ratio of T/T_t . Thus, the utility of the code is its capability to generate tables of compressible flow properties for any total conditions for any specified range of static temperatures ($T < T_t$, of course) or Mach numbers. In this section, the segments of the TPG code, Version 2.2, are described, code execution procedures are included, and examples of all user-supplied inputs are provided. The various types of output are also described.

The FORTRAN code, listed in appendix A, consists of a **Main** program, three **include** files, several subroutines, and a **Block Data** initialization routine and is designed to run on a minimally configured computer workstation. The subroutines are grouped according to purpose within several files and are called as needed from various locations within the **Main** program as well as from other subroutines. Table 1 summarizes the files and subroutines which comprise the TPG code. A Unix Makefile has been

Table 1. TPG Code Version 2.2 Files and Subroutines

Files	Contents
TPG.f	Main program
Version.h	Include code version identifier
params.h	Include parameters
dimens.h	Include common blocks
trangej.f	Subroutine trangej
cpsubs.f	Subroutines cpeval , cpNtgra , and cptNtgr
ntgrat.f	Subroutines intCp , and intCpT
titer.f	Subroutines tliter , and t2iter
Cratio.f	Subroutine Cratio
blockd.f	Block Data
initd.f	Subroutine initd

developed for compilation of the code and creation of an executable file. In the Unix environment, standard output prompts the user for the required input parameters for code execution, which are written to standard input. With one exception, all interactive inputs occur in the **Main** program. Defaults are provided for all inputs. A complete execution requires, at a minimum, an answer to each interactive prompt of a comma followed by a **carriage return**. Such a minimal execution generates a single output file containing a table of the basic gas expansion properties for the standard composition of air. Generation of more complete tables or files for postprocessing requires specific inputs, which will be described in the following sections.

Main Program

The first part of the **Main** program contains the interactive inquiries and responses which specify the gas components, the desired total temperature, the desired outputs, and the output formats. A typical example of code execution is shown in table 2 in which the user responses are italicized. A response of a comma indicates acceptance of a program default. Each user response is followed by a **carriage return** (not shown).

The first response required is an identifier character string (**ID**), or symbol name, for inclusion within the output files. The **ID** can have a maximum of 70 characters all entered on a single line; an **ID** that includes blank spaces must be enclosed in quotes. A default **ID** for air may be specified by a comma or the word **DEFAULT** (all uppercase or all lowercase letters); in this case, the next three questions are omitted and defaults are assumed. A particular database file may be specified next which describes the necessary thermochemical data for the gases of interest. The file name can have a maximum of 40 charac-

ters and quotes are not required on most computers. The contents of such a database file will be described in a later section. The code contains the database necessary to define a four-species mixture of air; this default is chosen by entering a comma. The gas mixture definition is completed by the third and fourth responses in which the number of individual species and the corresponding mass fractions are specified. Defaults may be selected at any time, and correspond to the standard composition of air. Regardless of the number of fractions, the code checks to see if the sum of the mass fractions equals unity and if the database contains sufficient information for the requested case. If the mass fractions do not sum to unity within a small tolerance, the code issues an error message and stops execution. If the sum is within unity plus or minus the tolerance, the last species fraction is recomputed so that the total is precisely unity and a warning message is output which describes the change. If the database contains insufficient information, an error message is output and execution is terminated.

The first two responses are sensitive to the case of the alphabetic character entered. That is, upper and lowercase alphabetic characters have unique meanings. However, all succeeding inputs are insensitive to case and either upper or lowercase responses have the same meaning within the code.

The next inputs define the composition and format of the table(s). The Total Temperature specifies the maximum possible upper temperature limit (for which the Mach number is zero). Following that, is an input that specifies whether the tables are to be in terms of static Temperature T or Mach number M increments. The default entries in the table(s) are given for incremental Mach numbers from an Initial Mach up to an Upper Mach number limit.

Table 2. Sample TPG Code Interactive Inputs

```

-----
|   Thermally Perfect Gas Properties Code   |
|                                     TPG, Version 2.2                                     |
|                                     |
-----

```

Enter the ID ('character string') for the gas mixture:

[default = 4-species Air]

'Air: containing standard mass fractions of N2, O2, Argon, and CO2'

Enter the name of the Database File for the Species properties:

,

Enter the number of species composing the mixture: [default = 4]

,

Enter the mass fraction, Y, of all 4 component species
in the order of the Database File (sum=1.0):

[defaults = 0.7553, 0.2314, 0.0129, 0.0004]

, , , ,

Enter the Total Temperature (in degrees K): [default = 400.]

1500.

Increment the table entries by constant Temp (K) or constant Mach number? (T/M)

[default = M]:

t

Enter the Initial Temperature, the Static Temperature Increment,
and the Low Temperature Limit (in degrees K):

[defaults = 1500., 10.0, 10.0]

1000., 20., 50.

Do you want to calculate the Normal-Shock Properties? (y/n): [default = N]

y

Enter the number of Tables to be output, 1 or 2 : [default = 1]

,

Enter the Tabular output location: screen=6, file=9 [default = 9 : TPG.out]

,

Do you want to output a TECPLOT file [TPGpost.dat] ? (y/n): [default = N]

y

Do you want to Ratio the data to the case of a
Calorically Perfect Gas ? (y/n): [default = N]

y

Enter the Calorically-Perfect Constant Gamma: [default=1.4]

1.4

Table 3. Sample **TPG.out** Header Information

<pre> Thermally Perfect Gas Properties Code TPG, Version 2.2 </pre>
<pre> Table of Thermally Perfect Gas Flow Properties Gaseous Mixture: Air: 4-Species Mixture of N2, O2, Argon, and CO2 Database file name: air.data Species Names are: N2 , O2 , Ar , CO2 , Species Mass Fractions are: 0.75530 0.23140 0.01290 0.00040 Species Mole Fractions are: 0.78092 0.20946 0.00935 0.00026 Mixture Properties: Molecular Wt. = 28.9663 Gas Constant = 2.87035E+02 J/(kg*K) Stagnation Temperature = 1500.000 (K) </pre>

Alternatively, if the constant Temperature option is specified, the table entries are for Static Temperature Increments from an Initial Temperature down to the Low Temperature Limit. The initial values are the total conditions by default. These inputs are separated by commas and any, or all, may be defaulted simply by entering a comma. Gas expansion properties are always included in the table and normal shock properties may be obtained by an answer *y* for “yes” to the inquiry. The relative locations of the expansion and shock property tables are determined by the answer to the next inquiry with regard to the number of tables (either 1 or 2). The normal shock properties may be output in the same table as the expansion properties in a wide format (158 character width), or may be output separately, in a second table cross-referenced to the first table of expansion properties by the Mach number and static temperature. The table of normal shock properties begins with sonic conditions and includes all subsequent (supersonic) entries. Because the tables can be rather extensive, they are written by default to an output file **TPG.out**. However, in response to the question of tabular output location, the tables could be written to standard output, which is typically the computer screen.

The next inquiries determine the output of additional files for data postprocessing and plotting. Because of extensive usage at NASA Langley Research Center, the Tecplot¹ (ref. 8) code format has been

chosen for these files. The format of this ASCII file, which is described in reference 8 and in appendix B, could be easily modified to satisfy the input requirements of many different graphics postprocessors. A single zone of information for all variables and all table entries is included. For subsonic conditions the normal shock properties have no physical meaning and are defaulted to a large negative number as a warning flag. The first postprocessor file **TPG-post.dat** contains the same basic data as that in the **TPG.out** tabular output. The second postprocessor file **TPGratio.dat** is generated only if a comparison of the thermally perfect properties to calorically perfect properties is desired. In this file all data are output as a ratio of thermally perfect values normalized by the corresponding calorically perfect values. A specific constant γ , which is required for the calorically perfect calculations, is the response to the final prompt. This last interactive input is the only one not requested from the **Main** or at the beginning of the interactive execution. The input is requested when and if the normalization calculation is about to begin.

Following the interactive inputs, the database file, if one is requested, is opened, read, and closed. Certain properties of the gas mixture are computed and the coefficients of the c_p relationship for the mixture are defined (eq. (7a)). The **TPG.out** file is opened and header information is written to it stating the gas mixture specifications and the total temperature. Sample header information is shown in table 3. Initialization of the case is completed by calculation of the sonic conditions as required by equation (44).

¹Tecplot: trademark of Amtec Engineering, Inc., Bellevue, WA 98009-3633.

A program loop for the temperature or Mach range between the desired limits computes the basic gas expansion properties. These properties are then output unless the single table format with the normal shock properties has been requested. A second loop for all supersonic Mach numbers calculates these normal shock properties. After the second loop is completed, the tabular output to **TPG.out** is completed and the file is closed. The same information is then output in postprocessor format to the **TPG-post.dat** file. Finally, normalization of the thermally perfect data with that of a calorically perfect gas is performed and the normalized results are output to the **TPGratio.dat** file. Execution of the code is completed by closing all files and recording warning summaries of the times the valid temperature ranges have been exceeded during the calculations. These warnings, if any, are related to the database information and are written to an additional file called **Extrap.WARN** for later reference.

Include (or Header) Files

The **Version.h** file contains a character variable which specifies the current version number of the computer code. This information is output at the beginning of each interactive execution and to the first lines of the **TPG.out** header.

Two files **params.h** and **dimens.h** contain information which determines the size of the computer memory required to execute the TPG code and, thus, the size of the case which may be specified. The dimensions of the primary arrays within the code as defined below are included in a FORTRAN parameter statement in **params.h** and have the following values as released in Version 2.2:

1. **mtrm** (=8) number of polynomial terms which define relationship for c_p/R
2. **mshpc** (=10) maximum number of gas species allowed
3. **mcvf** (=3) maximum number of temperature ranges per species allowed and corresponding sets of polynomial coefficients of equation (2)
4. **mtncr** (=10000) maximum number of computed static temperatures

All values assigned to the preceding parameters, except **mtrm**, may be changed at anytime to suit

particular user requirements. The code must then simply be recompiled and linked to form a new executable file. A change in **mtrm** may require code changes in the subroutines found in **cpsubs.f** which perform specific calculations using the $c_p(T)/R$ relationships. Changes to **mtrm** which are permitted without recoding the routines in **cpsubs.f** are described in "Polynomial Summation and Integration Subroutines."

The **dimens.h** file specifies common blocks containing all of the major arrays that are dependent on the parameters described above. Additional common blocks include the data for sonic conditions, certain species and mixture information, and several character variables.

FORTRAN **include** statements allow these header files to be separated from each FORTRAN routine so that the definitions are included at compile time as if the individual statements were within each routine. For example, the code dimensions need to be specified only once rather than in each routine.

Temperature Rangefinder Subroutine

The specification of any single function which can accurately describe the relationship between heat capacity and static temperature over a wide temperature range for typical gases is an extremely difficult task. However, when limited ranges are considered, maintenance of continuity and smoothness of separate functions at the limits of the individual ranges are much simpler. References 5 and 6 provide polynomial curve fits of the specific heat, specific enthalpy per degree, and specific entropy for a number of gases for multiple temperature ranges. The older report (ref. 6) includes a large selection of gases defined by five-term, fourth-order polynomials and listed as accurate for temperature ranges of 300 to 1000 K and 1000 to 5000 K. Continuity of the polynomials for each thermodynamic quantity was maintained at the common point of 1000 K. Appendix 2 of reference 5 contains updated polynomial expressions for a subset of the gases of reference 6. These updated polynomials contain eight terms and include all integer powers of T from -2 to 5 . The published temperature ranges for these polynomials are 200 to 1000 K and 1000 to 6000 K. Detailed information regarding the derivation and validity of these functions may be found in references 5 and 6.

To evaluate equation (7a) for specific heat at a given temperature, the appropriate temperature range is required; the **trangej** subroutine was developed to provide this. Given a particular temperature, the routine searches to determine the correct

temperature range from the set of valid ranges for the gas mixture. For a temperature beyond the limits of any range, the closest range is specified for extrapolation and a warning message is output to the file **Extrap.WARN** for that particular temperature. A single extrapolation warning message is written at the end of the **TPG.out** file which notes the temperature below which extrapolations were performed. This warning message appears when any of the component species of a gas mixture requires extrapolation.

Polynomial Summation and Integration Subroutines

The equations defined in the derivation section require evaluation of c_p , the integral of c_p , and the integral of c_p/T . These evaluations are performed numerically in three subroutines contained in file **cpsubs.f**. These three subroutines contain code specific to the form of the polynomial expression of equation (2): the **cpeval** subroutine evaluates c_p as a function of T from equation (7a), the **cpNtgra** subroutine evaluates the integral of c_p for the range of T to T_t from equation (18), and the **cptNtgr** subroutine evaluates the integral of c_p/T for the range of T to T_t from equation (35). Required inputs to the integration subroutines are the mixture polynomial coefficients, the static temperature, and the total temperature.

For integrations that cover multiple temperature ranges, **cpNtgra** and **cptNtgr** must be called once for each temperature range and the corresponding set of coefficients. This function is performed in the TPG code by two subroutines **intCp** and **intCpT** in the file **ntgrat.f**. Individual results of calls to the **cpNtgra** and **cptNtgr** subroutines are summed to yield a total integral. The **trangej** subroutine determines the ranges which include T and T_t . The total integral is divided into separate integrals as follows:

$$\int_T^{T_t} c_p dT = \int_T^{T_{\text{lim}}} c_p dT + \int_{T_{\text{lim}}}^{T_t} c_p dT \quad (60)$$

This decomposition of the single integral is then performed as required to cover all of the temperature ranges.

The **cpeval**, **cpNtgra**, and **cptNtgr** subroutines assume a polynomial expression of the form given in equation (7a). The lowest power of T is -2 . The highest power of T must be at least 2, which requires the parameter **mtrm** ≥ 5 . Any **mtrm** ≥ 5 may be set in **params.h** with no changes required in the FORTRAN code. However, for **mtrm** < 5 or a

different expression for c_p/R , these three subroutines must be modified. An increase of **mtrm** beyond the code release value of 8 would include higher order powers of T in the polynomials.

Nonlinear Iteration Subroutines

As stated previously, the properties at sonic conditions must be known in order to compute the value A_1/A_* for any T_1 . A combination of equations (19), (20), and (21) gives the relationship for T_1 as

$$2 \int_{T_1}^{T_t} c_p dT = M_1^2 \gamma_1 R T_1 \quad (61)$$

for any M_1 , in which γ_1 is a function of T_1 . At sonic conditions $M_1 = M_* = 1$ by definition and equation (61) becomes equation (45). An application of Newton's method (ref. 9) to equation (61) yields an iterative technique for T_1 that has been implemented in subroutine **t1iter** (file **titer.f**). The derivative in Newton's method is defined by a first-order finite difference expression rather than by an analytic expression. For the iterative solution of this well-behaved function, an initial guess of $T_1 = 0.8 * T_t$ was satisfactory. The algorithm is called once in the TPG code to determine the static temperature at sonic conditions; however, the algorithm is actually valid for determining the static temperature for any Mach number, not just M_* . Therefore, **t1iter** is also called for each Mach number tabular entry when the Mach number increment option is selected.

Subroutine **t2iter** also implements a Newton iteration to solve equation (51) for the static temperature T_2 behind a normal shock. This function is not as well-behaved as that for T_1 and tends to become rather flat near the minimum. The solution by Newton's method either converges slowly or becomes unstable; for some conditions, desirable levels of convergence cannot be attained. Checks on the magnitude of the derivative and the number of iterations have been implemented in the code to prevent divergence; the desired convergence tolerance is increased, if needed, to prevent divergence. A warning message is written to standard output each time this tolerance is changed. For maximum stability, the iteration is started with an initial guess defined by the minimum of either $T_2 = 0.99 * T_t$ or the calorically perfect value based upon local conditions.

One of the arguments for each Newton subroutine is the desired convergence tolerance **epsil**. The tolerance is set in a **Main** program **data** statement at an acceptable value for a computer word size of 32 bits. For computers that use a different word size

(e.g., a CRAY² with a 64-bit word), this tolerance may be changed for improved accuracy or stability.

Calorically Perfect Comparison

Subroutine **Cratio** is called after all gas properties have been computed from the thermally perfect relationships. With the last user input γ , this subroutine applies the appropriate equations from NACA Rep. 1135 to compute corresponding gas properties for a calorically perfect gas. Each property computed by the thermally perfect equations is normalized by the calorically perfect value to allow analysis of the magnitude of the thermal dependency. Ratios of physically meaningless values, such as normal shock properties at subsonic values of M_1 , are set to defaults of large negative numbers in Version 2.2 of the code. The ratios are output to the file **TPGratio.dat** for postprocessing in the Tecplot format described in appendix B. Again, this format can be easily changed to suit the needs of a different postprocessor. All file formats are included in **Cratio**.

Data Initialization

Data initialization is located in three places within the TPG code. A **Block Data** subroutine contains **data** statements which initialize the variables associated with individual species and the gas mixture. Most of the **Block Data** is associated with the default database information for the standard composition of air. A second set of **data** statements are included within the **Main** program itself. These statements set defaults for the variables that do not need to be passed to subroutines via common blocks such as the universal gas constant, the sonic Mach number, the Newton iteration convergence tolerance, and a finite representation of infinity for numeric output. Additionally, the default responses for several of the interactive inputs (particularly the default yes or no answers) are set in the **Main data** statements.

The third location for data initialization is in the subroutine **initd** where the arrays of gas properties are set to defaults. The TPG code could be modified to allow the user to redefine the total temperature, the temperature or Mach increments, and/or the temperature or Mach limits, and then recompute the tables for a given mixture within a single execution. For such a modification, all the necessary arrays could be reset to their defaults by a single subroutine call.

Database File Format

The thermochemical data required by the TPG code for a given mixture of gases are defined in a database file to be read at execution time. As previously stated, a database for the standard composition of air is contained within the code and may be accessed as the default. However, for mixtures of other gases or more complete models of air, a separate database file may be provided. The format is simple; a two-line data file header is followed by groups of data for each species. A sample two-species database is shown in table 4, and specific database files are included with the discussions of the test cases to follow.

The first line is a descriptor of the data to follow on the second line and, as such, is not actually read by the TPG code. Those data consist of the number of species for which the file includes thermochemical data and the number of temperature ranges for which separate polynomials define c_p/R as a function of T . These integer values are read in free format and are separated by one or more blanks. Version 2.2 of the code requires that, for each species within a particular file, each of the polynomials must have the same limiting temperatures for each range, except for the absolute minimum and maximum temperatures of the overall definition. That is, if the polynomials for one gas are valid from 200 to 1000 K, and from 1000 to 5000 K, then each gas within that database file must also be defined by one polynomial up to 1000 K, and a second one above 1000 K. The absolute extrema of 200 and 5000 K are not required to be identical since the code simply extrapolates the polynomials beyond these limits. Extrapolation warnings are based upon the worst case extrema of the most conservatively defined gas. The requirement that all of the temperature ranges coincide is not a limitation of the basic algorithm but only of Version 2.2 of the code. (Note that this limitation can be easily overcome by splitting any particular temperature range into multiple consecutive ranges with identical coefficients.)

The next set of lines are repeated for each of the gaseous species in the file; the number of individual gaseous species expected by the code is given in the second line. Error handling has been incorporated within the code to recognize **End-of-File** on most computers without terminating execution, (i.e., the case in which the actual number of species defined is less than expected). However, some computers and/or FORTRAN compilers may not function properly if the header information and the actual number of gases do not agree.

²Cray Research, Inc., Minneapolis, MN 55402.

Table 4. Sample Thermochemical Database File

```

# of species  # of Temperature ranges:  NASP TM 1107 + Mods.
  2              2
Name:  Molecular Wt.
N2      28.0160
tmin    tmax
20.     1000.
Cp/R Coefficients:c1(-2)-->c1(5)
-1.33984200E+01 1.34280300E+00 3.45742000E+00 5.74727600E-04
-3.21711900E-06 7.50775400E-09 -5.90150500E-12 1.50979900E-15
tmin    tmax
1000.   6000.
Cp/R Coefficients:c2(-2)-->c2(5)
5.87702841E+05 -2.23921563E+03 6.06686971E+00 -6.13957913E-04
1.49178026E-07 -1.92307130E-11 1.06193594E-15 0.00000000E+00
Name:  Molecular Wt.
O2      32.0000
tmin    tmax
30.     1000.
Cp/R Coefficients:c1(-2)-->c1(5)
3.88517500E+01 -2.70630800E+00 3.56119600E+00 -3.32782400E-04
-1.18148000E-06 1.10853500E-08 -1.49299400E-11 5.99553800E-15
tmin    tmax
1000.   6000.
Cp/R Coefficients:c2(-2)-->c2(5)
-1.05642070E+06 2.41123849E+03 1.73474238E+00 1.31512292E-03
-2.29995151E-07 2.13144378E-11 -7.87498771E-16 0.00000000E+00

```

The thermochemical data for the first gas begins with the third line of the file, which is the descriptor for the next line of data. The fourth line contains the name of the gas (five characters), one or more blanks, and its molecular weight. Each polynomial definition follows beginning with the lowest temperature range. Line six specifies the minimum and maximum temperatures for the first polynomial. After another descriptor line, the coefficients A_1 to A_8 (or A_{mtrm} if $\text{mtrm} \neq 8$) for the polynomial are tabulated, in free format separated by blanks or on multiple lines. After a descriptor line, the minimum and maximum temperatures for the second polynomial are specified next, followed by a descriptor line and a second set of tabulated coefficients. This pattern is repeated for all the temperature ranges specified in the database header. The data for a second gas follow directly after these lines in the same format as the first and continue in this pattern until all gases have been defined.

The TPG code will use the gas definitions in the order specified within the database file and the user must input mass fractions in that same order. However, mass fractions of zero are acceptable inputs

if one or more of the leading species within a given file are to be omitted. Also, the polynomial coefficients for a particular gas do not all have to be nonzero. In particular, a calorically perfect gas may be defined by a database in which all of the coefficients are zero except A_3 , which equals the caloric constant for c_p/R .

TPG Code Validation

Calorically Perfect Temperature Regime

The first validation test of the TPG code was the verification of accuracy in the calorically perfect temperature regime in which air is the test gas. In this temperature regime, the specific heat of air is nearly constant and therefore the TPG code results should be nearly identical to the tables of NACA Rep. 1135. For this test case, the default data file for standard four-species air was used (table 5) along with the default (standard) values for the mass fraction composition of air. The code default total temperature of 400 K, which is well within the calorically perfect temperature regime for air, was selected and the case was run with the TPG code in the temperature increment mode. The upper temperature limit

(Initial Temperature) was defaulted to the total temperature. The Static Temperature Increment and Low Temperature Limit were chosen to be 2 K and 20 K, respectively. (The Static Temperature Increment merely determined the number of rows of tabulated output in the **TPG.out** file. The choice for a Low Temperature Limit determined the maximum Mach number presented in this file.) The **TPG.out** file for this test case is given in table 6(a). Table 6(b) shows the results for the same test case obtained with the Mach number increment option of the TPG code. A Mach number increment of 0.05, a minimum Mach number of 0.0 (the default value), and a maximum Mach number of 10.0 were selected for this case. A comparison of table 6(b) with tables I and II from NACA Rep. 1135 for any matching Mach number shows the desired agreement and validates the TPG code in this calorically perfect temperature regime. The small differences that are observed between the corresponding values of table 6(b) and the tables of NACA Rep. 1135 are in either the third or fourth digit. To better examine these small differences, the TPG code generated the ratio of the gas properties calculated with the thermally perfect relations (tables 6(a) and 6(b)) to those calculated from the calorically perfect relations (tables of NACA Rep. 1135). These results have been plotted versus Mach number in figures 1 and 2. From these figures, the maximum difference between the values listed in table 6(b) and the tables of NACA Rep. 1135 appears to be approximately 0.5 percent. Note that these small differences actually represent the small amount of error associated with the tabulated values of NACA Rep. 1135 which resulted from the calorically perfect gas assumption. Close inspection of table 6(a) or table 6(b) reveals that a slight variation with temperature actually exists in the specific heat ratio, which leads to the noted differences when compared with the calorically perfect gas properties.

Thermally Perfect Temperature Regime

The first step in verification of the TPG code in the thermally perfect temperature regime was to compare the γ variation for air computed by the TPG code with both the γ variation calculated from NACA Rep. 1135 (eq. (180)) and the theoretical thermally perfect γ variation from reference 4 obtained with the theoretical c_p data for N_2 , O_2 , Ar, and CO_2 . The variation of γ as a function of temperature is presented in figure 3. Below 300 K, γ values predicted by NACA Rep. 1135 have attained their asymptotic value of 1.400 while the γ values predicted by the TPG code have reached a slightly greater asymptotic value of 1.401, which is in agreement with the theoretical data. Above 300 K, both the TPG code and

the exponential expression for γ in NACA Rep. 1135 produce nearly identical γ variation that is in excellent agreement with the theoretical γ values up to approximately 1600 K; at this point, the γ curve of NACA Rep. 1135 begins a gradual divergence away from the TPG code curve of γ and the theoretical results. This divergence results from the inability of the exponential expression of NACA Rep. 1135 (essentially a single constant Θ exponential curve fit) to accurately model the true thermally perfect behavior of the gas at the higher temperatures. The TPG code avoids this limitation by utilization of multiple-range polynomial curve fits to model the variation of specific heats; this particular application of the code consisted of two eight-term, fifth-order polynomial curve fits. From a true gas behavior standpoint, neither NACA Rep. 1135 nor the TPG code predicts an accurate γ variation for air above 1600 K because of the effects of dissociation. A discussion of this temperature limitation associated with the application of the TPG code is presented in the next section.

The remaining gas properties computed by the TPG code in the thermally perfect temperature regime were verified for test cases at total temperatures of 556 K (1000° R), 1111 K (2000° R), 1667 K (3000° R), and 2778 K (5000° R) for air (standard four-species composition) as the test gas. These four specific test cases were selected so that a comparison could be made with the caloric imperfection charts of NACA Rep. 1135 which give the compressible flow gas properties for air computed from the thermally perfect relations based upon equation (1) of this paper. Each chart from NACA Rep. 1135 shows the variation of one gas property, as normalized by its calorically perfect value, versus Mach number for the above mentioned four total temperatures. The TPG code results for these four test cases were also normalized by their calorically perfect values and then plotted together with the results from the caloric imperfection charts of NACA Rep. 1135. (The results of NACA Rep. 1135 have been regenerated here for plotting purposes from the appropriate equations in ref. 1.) Figures 4–15 present the results of the TPG code and NACA Rep. 1135 and correspond to charts 9–20, respectively, from reference 1. Examination of figures 4–15 shows that overall agreement (maximum difference less than one percent) exists for the compressible flow properties computed from the two different methods. The small differences that are observed in these figures can be attributed in most cases to one of the two sources of γ inaccuracies noted previously. The predominate difference noted in figures 4–15 is between the curves of the TPG code and NACA Rep. 1135 for the test case at a total

temperature of 2778 K (5000° R). This difference is discernible from the start of the expansion (clearly evident in figs. 4, 8, and 12) and continues throughout the Mach number range. This results from the difference in the predicted γ values between the two methods for the temperature above approximately 1600 K. (See fig. 3.) The other noticeable difference between the curves of the TPG code and NACA Rep. 1135 occurs at the total temperatures of 1667 K, 1111 K, and 556 K. At some given value of Mach number, the curves of the TPG code diverge from the asymptotic plateau value of NACA Rep. 1135. This divergence is most apparent in figures 6–9, and 15. The onset of divergence begins at approximately $M = 3$ for $T_t = 556$ K, at $M = 5$ for $T_t = 1111$ K, and at $M = 6$ for $T_t = 1667$ K. Examination of the **TPG.out** files for these test cases (not included in this report) revealed that the Mach numbers at this onset of divergence for the above three test cases all correspond to a static temperature value of approximately 200 K. The divergence of the curves of the TPG code and NACA Rep. 1135, which is discernible in the plotted data at about 200 K, is actually a consequence of the difference in the predicted γ values as shown in the low-temperature range of figure 3. This comparison verifies the TPG code accuracy with the derived thermally perfect gas relations based upon polynomial expressions for c_p . Although these test cases were all for air, which is a primarily diatomic gas, the TPG code is also valid for polyatomic gases. The utilization of a polynomial curve fit for c_p makes the TPG code applicable to any molecular structure of the gas.

As a verification of the above statement, figure 16 presents the γ variation for a triatomic molecule CO_2 predicted by the TPG code versus the theoretically thermally perfect γ variation from reference 4. Unlike figure 3, there is no γ curve from NACA Rep. 1135 because its equation (180) is not valid for a triatomic molecule such as CO_2 . The agreement in the γ variation in figure 16 is excellent, which is just a confirmation of the curve fit for c_p as a function of the temperature utilized by the TPG code. Table 7 gives the **TPG.out** file for this CO_2 test case. (Note that for the CO_2 test case, the **air.data** database file was used with the mass fractions for N_2 , O_2 , and Ar set equal to zero.)

Temperature Boundaries for Application of TPG Code

The TPG code will provide valid results as long as its application is kept within the thermally perfect temperature regime for the gas of interest. If the code is used outside of the region for which c_p

is a function of temperature only, then the thermally perfect results produced by this code will no longer accurately reflect what actually occurs in nature. To illustrate what happens outside the boundaries of the thermally perfect temperature regime, comparisons have been made with air data from NBS “Tables of Thermal Properties of Gases.” (See ref 3.) Figure 17 presents the variation of specific heat (nondimensionalized by the gas constant) with temperature for air up to 3000 K. This figure contains data from the TPG code, NACA Rep. 1135 (eq. (178)), and reference 3. The results of the TPG code and NACA Rep. 1135 are nearly identical; the NBS data (plotted for three pressures of 0.1, 1.0, and 10 atm) coincide with the other results only between approximately 500 K and 1500 K. Above 1500 K, the NBS data yields significantly larger values of c_p/R and clearly becomes a function of pressure as well as temperature. This phenomenon is a result of dissociation effects. Below 500 K, the NBS curve for 10 atm diverges to greater values of c_p/R . In this region of relatively low temperatures and high pressures, real gas effects are the cause of this deviation from the thermally perfect behavior. (Here the term *real gas* refers to a gas for which the intermolecular forces are not negligible.) From reference 3, examination of the compressibility factor table for air in this range of temperature and pressure verifies this conclusion. (Note that at low temperatures and also relatively low pressures, the thermally perfect results will accurately predict the actual behavior of the gas properties.) The heat capacity information given in figure 17 is presented in an alternate form in figure 18, which shows the variation of the ratio of specific heats with temperature for air from the same three sources. The characteristics discussed above are also observable in this figure. These two figures emphasize that the TPG code user must remain aware of the low- and high-temperature boundaries associated with the thermally perfect assumption for the particular gas under consideration. (Note that the user should not confuse the above issue with the extrapolation warnings which result from exceeding the limits of application of a particular curve fit for c_p/R as a function of T .)

Additional Sample Cases

Although only air and CO_2 test cases have been presented thus far, the TPG code has the potential to produce tables of compressible flow properties for any gas or any mixture of gases for which the required polynomial curve fit information for c_p is available. Four additional sample cases have been included in this section to provide a better understanding of the full capability of the TPG code. The four gases are

steam, a mixture of steam and air, a mixture of tetrafluoromethane and argon, and nitrogen, which are examples of monatomic, diatomic, triatomic, and polyatomic gases. The database files for these four sample cases are given in tables 8–11. Tables 12–15 are the **TPG.out** files which contain the tabulated output of compressible flow gas properties for these four sample cases. The values of mass fractions and the stagnation temperatures were arbitrarily selected for all four cases. Stagnation temperature values were checked to ensure that they were safely below the temperature limits for all component species at which dissociation effects would invalidate the thermally perfect assumption. The low-temperature limit in all cases was simply selected as the **tmin** value of the lowest temperature range curve fit for c_p/R . For the multiple gas species sample test cases, the highest low-temperature range **tmin** values were selected as the low-temperature limit. This ensured that no curve fit extrapolations would be encountered.

A verification that the results from the low-temperature region of tables 12–15 are not in the region of real gas effects cannot be performed until a value of total pressure is specified. This value determines the magnitude of the static pressures from the **TPG.out** file. In the case of a mixture of gases, the value of static pressure for the mixture needs to be divided into the values of partial pressures for the component gas species by application of the mole fraction information printed in the header of the **TPG.out** file. From the combination of static temperature and pressure for each component gas species, the compressibility factor Z is obtained from a source such as reference 3, which provides tables of compressibility factors for several gas species. If the value for Z differs by more than one percent from unity, then real gas effects should be considered if accurate results are desired. A check to determine if liquefaction of the gas has occurred for the given static temperature and pressure is also appropriate at this stage in the analysis. The possibility of liquefaction exists when the compressibility factor table does not provide data at the desired ranges of low temperature and high pressure. A table or plot of the vapor pressure versus temperature will verify whether the particular component species is in either the liquid or gas phase.

Conclusions

A set of compressible flow relations for a thermally perfect gas has been derived for a value of c_p expressed as a polynomial function of temperature and developed into a computer program referred to as the TPG code. The code produces tables of compressible flow properties similar to those found in NACA Rep. 1135. Unlike the tables of NACA Rep. 1135 that are valid only in the calorically perfect temperature regime, the TPG code results are also valid in the thermally perfect temperature regime, which gives the TPG code a considerably wider range of temperature application. Accuracy of the TPG code in the calorically perfect temperature regime was verified by comparisons with the tables of NACA Rep. 1135. The small differences observed in this comparison were identified as an inaccuracy of the tabulated values in NACA Rep. 1135 that resulted from the calorically perfect gas assumption. In the thermally perfect temperature regime, the TPG code was verified by comparisons with results obtained from the method of NACA Rep. 1135 for calculation of thermally perfect compressible flow properties. The TPG code is applicable to any type of gas and is not restricted to only diatomic gases as is the method of NACA Rep. 1135. In addition, the TPG code can accept any specified gas mixture for which the component gas species polynomial curve fit information for c_p is known because the calculation of the pertinent thermochemical mixture properties is performed within the code.

The temperature limits for application of the TPG code have also been examined. The thermally perfect behavior of any gas species will terminate at some combination of low temperature and high pressure due to the presence of real gas effects and at some value of high temperature due to dissociation (except for monatomic gases). Beyond these temperature limits, the TPG code may no longer accurately predict the actual behavior of gas properties. However, within the temperature range in which the thermally perfect assumption is valid, the TPG code provides accurate gas species or gas mixture compressible flow properties.

NASA Langley Research Center
Hampton, VA 23681-0001
May 3, 1994

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Appendix B

Tecplot ASCII Output File Formats

The TPG code output data files for postprocessing are in the Tecplot ASCII format defined in reference 8 and summarized below. This format was chosen for its simplicity and current widespread usage at NASA Langley Research Center. The Tecplot interactive plotting program, developed by Amtec Engineering, Inc., provides a suitable means for visualization of the tabular results of the TPG code. However, the output file formats could be easily modified for compatibility with many other graphics post-processing software packages; and the ASCII output format facilitates the transfer of data between various computer platforms. The following discussion will be useful in the conversion process.

The TPG output files which utilize this format are the **TPGpost.dat** and the **TPGratio.dat** files. **TPGpost.dat** contains the basic properties of the thermally perfect gas, which are also output to the **TPG.out** file. A sample **TPGpost.dat** file is shown in table B1. The **TPGratio.dat** file contains the same basic properties but in the form of ratios with the properties of a corresponding calorically perfect gas. The ratio of specific heats of the calorically perfect gas is one of the interactive inputs at the time of TPG code execution.

The first line in each of these postprocessor data files is a **TITLE** record containing the **ID** for the corresponding TPG calculation. A record designation **TITLE =** precedes the data title; a sample **TITLE** record for the default data is shown in the table. The **ID** is entered as part of the interactive input and is the portion within the double quotes.

The second line in the postprocessor files contains the names of the variables to be included, and also the number of variables for which data are included in the file. A record designator of **VARIABLES =** precedes the list of names. The current version of Tecplot restricts the length of each name to five characters. The names in the **TPGpost.dat** file (and the data to follow) are listed in the same order as found in the basic **TPG.out** tabular listing. The **TPGratio.dat** file utilizes the same names and order, except that the variables T_1 and $\beta = \sqrt{|M_1^2 - 1|}$ are omitted. Because the caloric data are not a function of temperature, the Mach number is identical for both calorically and thermally perfect flows. The variable names are abbreviated forms of the heading names for the columns of tabulated data listed

in **TPG.out**. For example, all variables which are ratios have the / omitted from the name. Pressure, temperature, and density (**RHO**) variables utilize single uppercase letters to designate the function (i.e., **P**, **T**, and **R**). The dynamic pressure is represented by **q**. A lowercase **t** represents the subscript **t** for total, or stagnation, conditions. The conditions upstream and downstream of a shock are signified by the numerals 1 and 2, respectively; the 1 is occasionally omitted for brevity. The letters **str** for * denote sonic conditions. The same variable names are used in both **TPGpost.dat** and **TPGratio.dat**; however, the values within **TPGratio.dat** are ratios with respect to calorically perfect gas calculations. The **VARIABLE** record in the **TPGpost.dat** file thus appears as shown in the second line in the table. If the normal shock properties are not computed, the last six variables are omitted.

The third line of the files (table B1) is referred to as a **ZONE** record. A ten character zone title, identified by **T=**, follows the record designator **ZONE**. The TPG zone title contains the total temperature for which the data were computed. The number of data points **I=** recorded within the file follow the zone title. Although the Tecplot format allows **IJ**-ordered data sets, the TPG code output requires only the single **I** index. Therefore, the next data output is fixed for all cases as **J=1**. The last information on the **ZONE** record describes the order in which the data that follow are listed. The **F=POINT** signifies that the data are presented in variable sequence first. That is, for each Mach number and/or temperature data point, the **N** variables are listed sequentially, followed by the **N** variables of the next Mach number and/or temperature data point.

The actual gas property data follow the three header lines. The data are written in FORTRAN exponential format with six significant digits; the page format provides up to a maximum of eight values per line. Thus, when normal shock data is included, the sixteen values require exactly two successive lines in **TPGpost.dat**. Successive Mach number and/or temperature data points always begin on new lines. Data values are output for every variable at each data point. Data values for the normal shock relations at subsonic Mach numbers (which have no physical meaning) are defaulted to a large negative number as a warning flag. This flag is intended to help the user recognize and avoid plotting these results. The flag magnitudes are set in the **initd** subroutine for **TPGpost.dat** and in subroutine **Cratio** for **TPGratio.dat**.

Table B1. Sample **TPGpost.dat** File

```

TITLE = "Air: 4-Species Mixture of N2, O2, Argon, and CO2"
VARIABLES = M1 , T1 , Gamma, PiPt, RiRt, TiTt, Beta, q1Pt, AAstr, VAstr, M2 , P2P1, R2R1, T2T1, Pt2Pt,
            PiPt2
ZONE T="Tt= 2000.", I= 6, J= 1, F=POINT
0.00000E+00 2.00000E+03 1.29801E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 0.00000E+00
9.99990E+07 0.00000E+00 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07
5.93104E-01 1.90000E+03 1.30003E+00 8.00246E-01 8.42364E-01 9.50000E-01 8.05126E-01 1.82981E-01
1.20218E+00 6.19233E-01 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07
8.59855E-01 1.80000E+03 1.30225E+00 6.33527E-01 7.03919E-01 9.00000E-01 5.10538E-01 3.04987E-01
1.01864E+00 8.74541E-01 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07 -9.99990E+07
1.00000E+00 1.73804E+03 1.30376E+00 5.44935E-01 6.27069E-01 8.69019E-01 0.00000E+00 3.55233E-01
1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 5.44935E-01
1.08104E+00 1.70000E+03 1.30474E+00 4.95617E-01 5.83079E-01 8.50000E-01 4.10660E-01 3.77853E-01
1.00554E+00 1.06954E+00 9.26497E-01 1.19181E+00 1.14390E+00 1.04189E+00 9.99393E-01 4.95919E-01
1.28333E+00 1.60000E+03 1.30754E+00 3.82658E-01 4.78322E-01 8.00000E-01 8.04318E-01 4.12012E-01
1.06318E+00 1.23309E+00 7.91595E-01 1.73683E+00 1.52015E+00 1.14254E+00 9.81353E-01 3.89929E-01

```

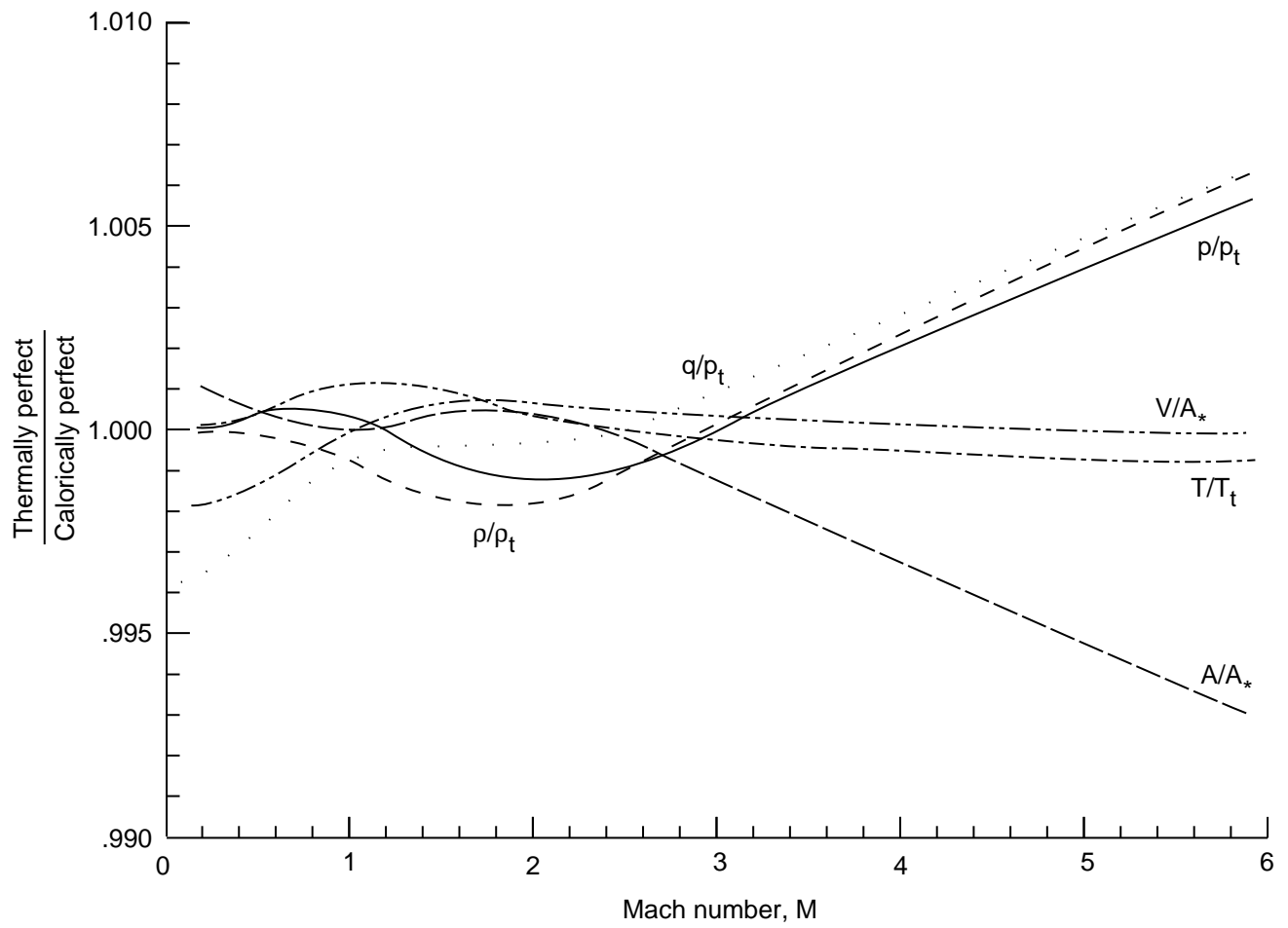


Figure 1. Effect of caloric imperfections on gas expansion properties ($T_t = 400$ K).

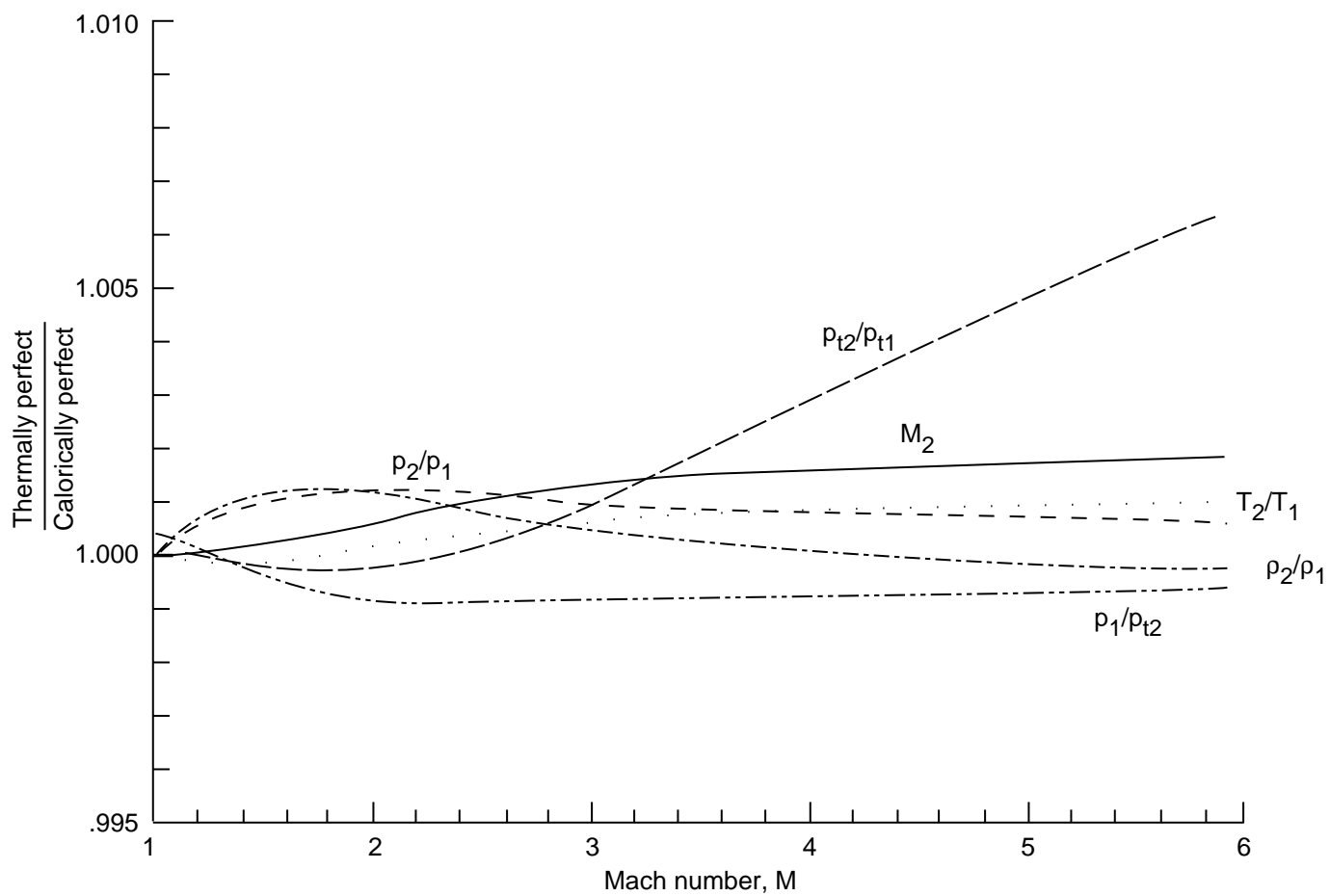


Figure 2. Effect of caloric imperfections on normal shock properties ($T_t = 400$ K).

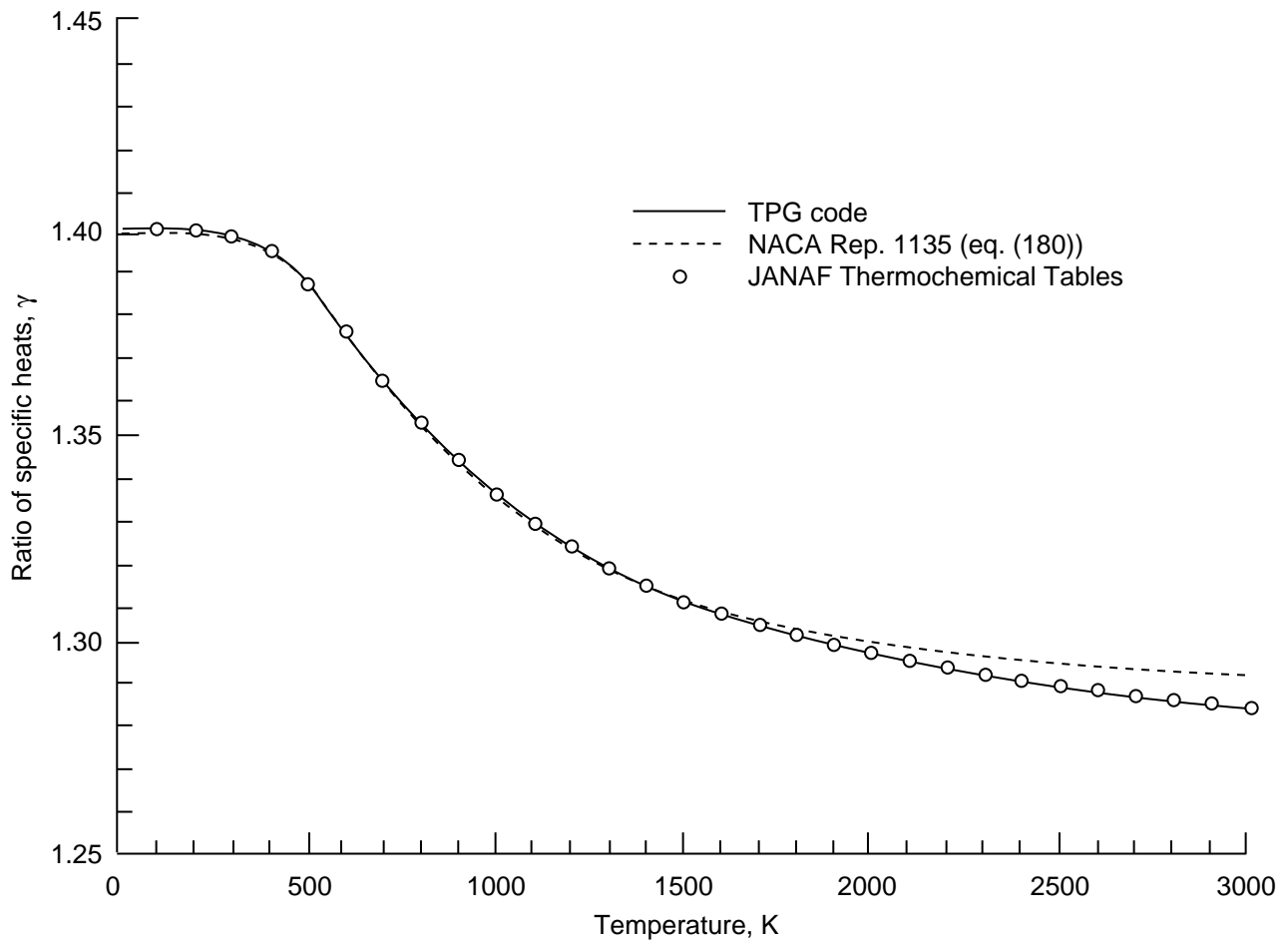


Figure 3. Variation of ratio of specific heats with temperature for thermally perfect air.

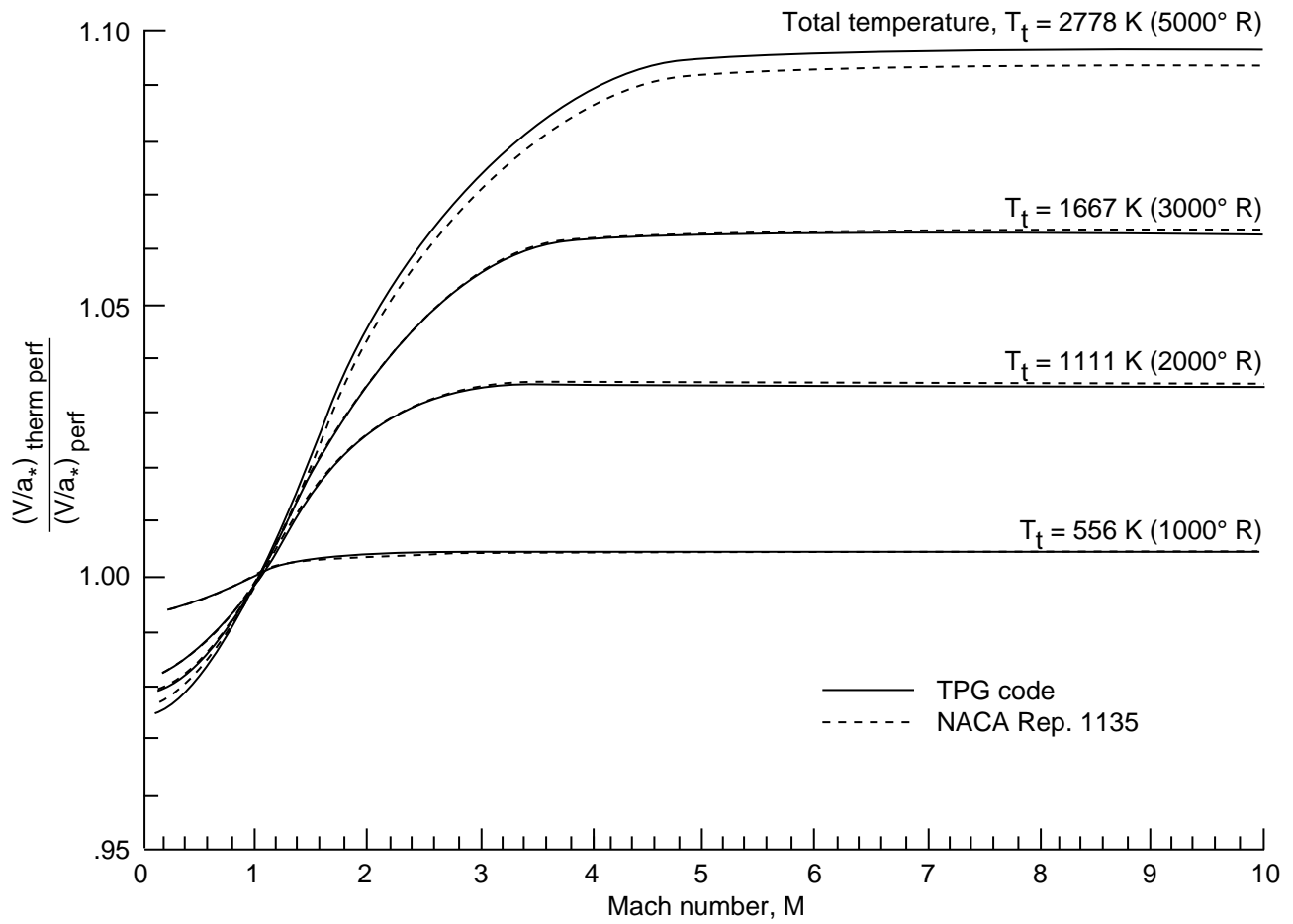


Figure 4. Effect of caloric imperfections on ratio of local speed to speed of sound at $M = 1$.

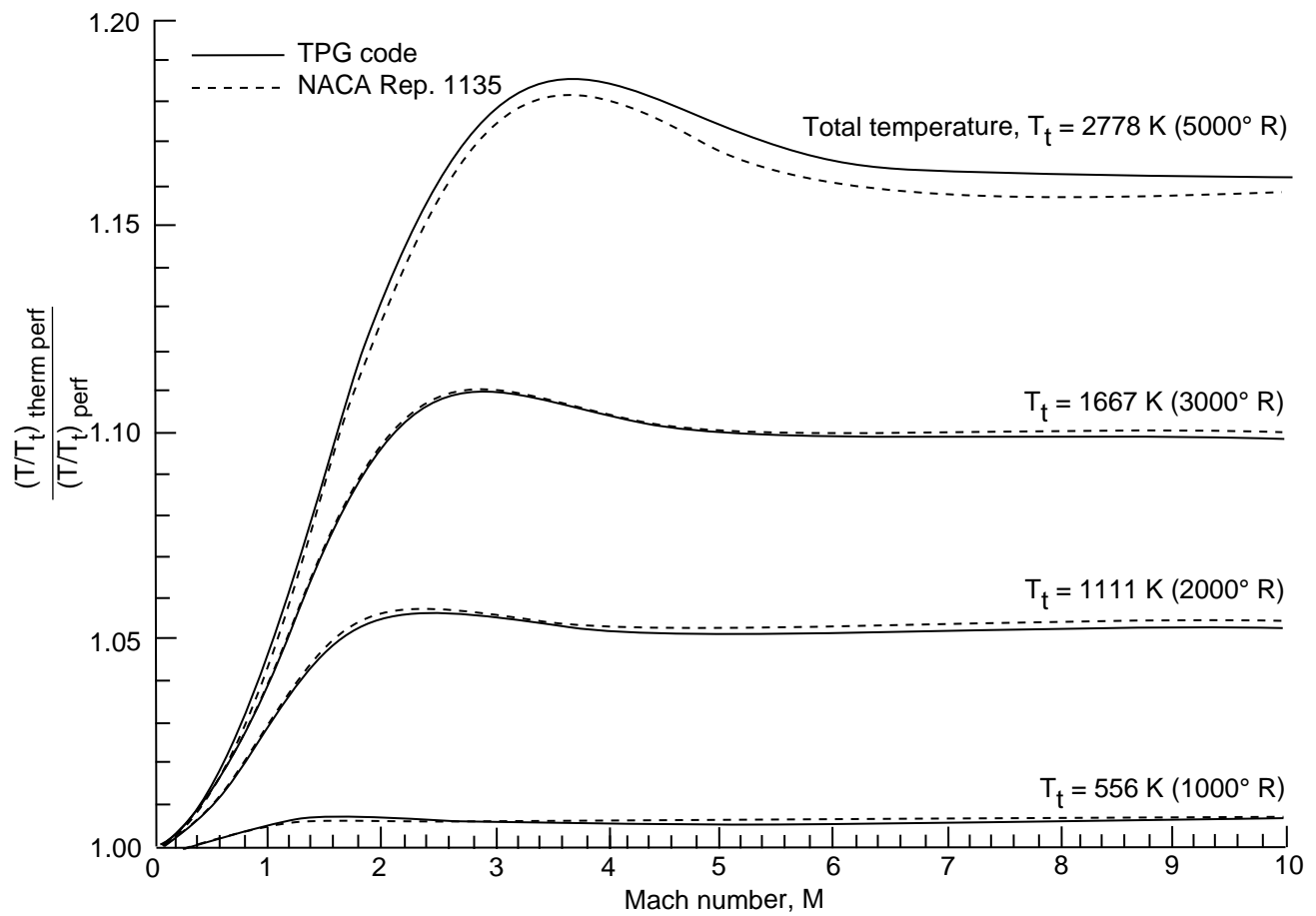


Figure 5. Effect of caloric imperfections on ratio of static temperature to total temperature.

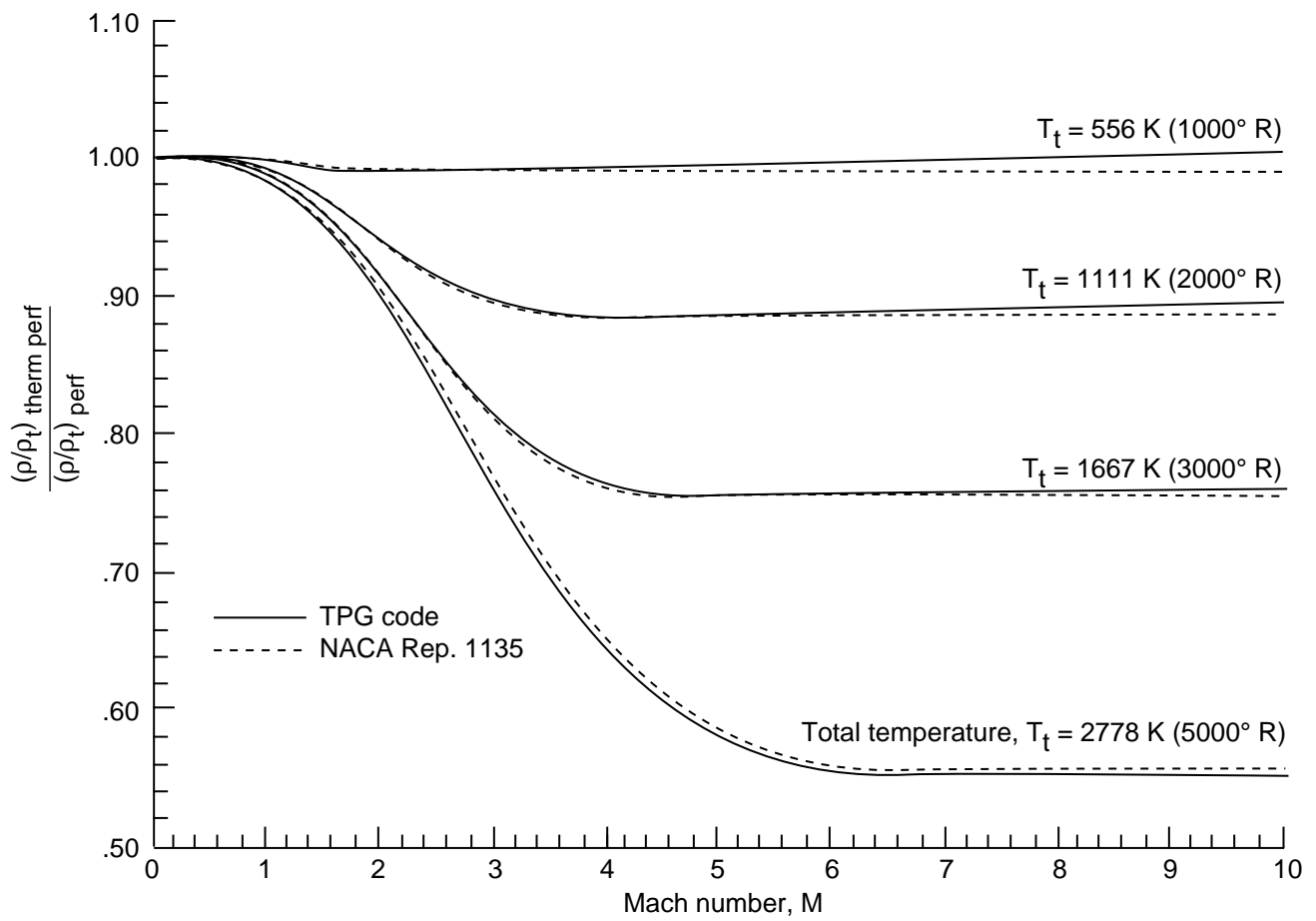


Figure 6. Effect of caloric imperfections on ratio of static density to total density.

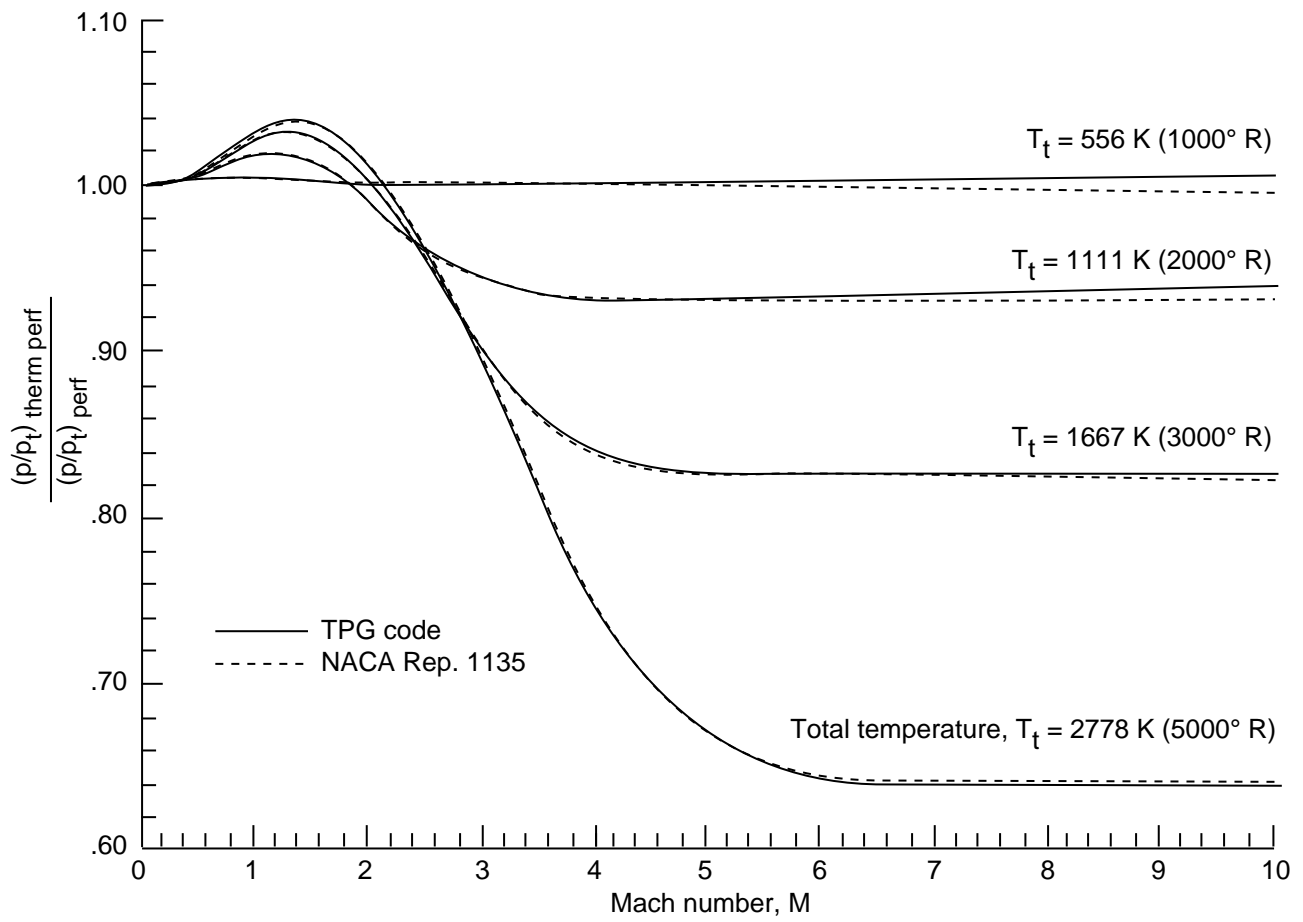


Figure 7. Effect of caloric imperfections on ratio of static pressure to total pressure.

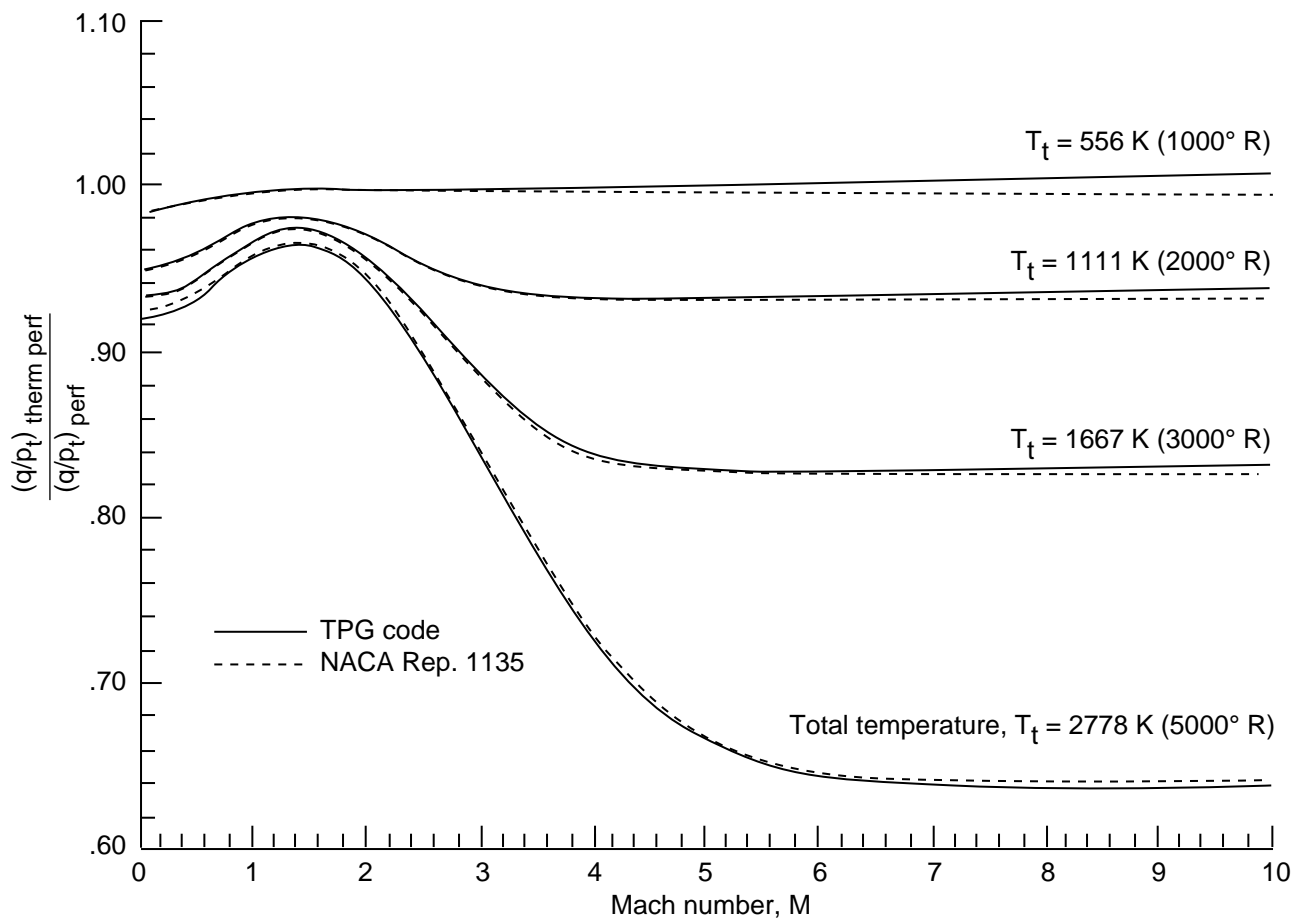


Figure 8. Effect of caloric imperfections on ratio of dynamic pressure to total pressure.

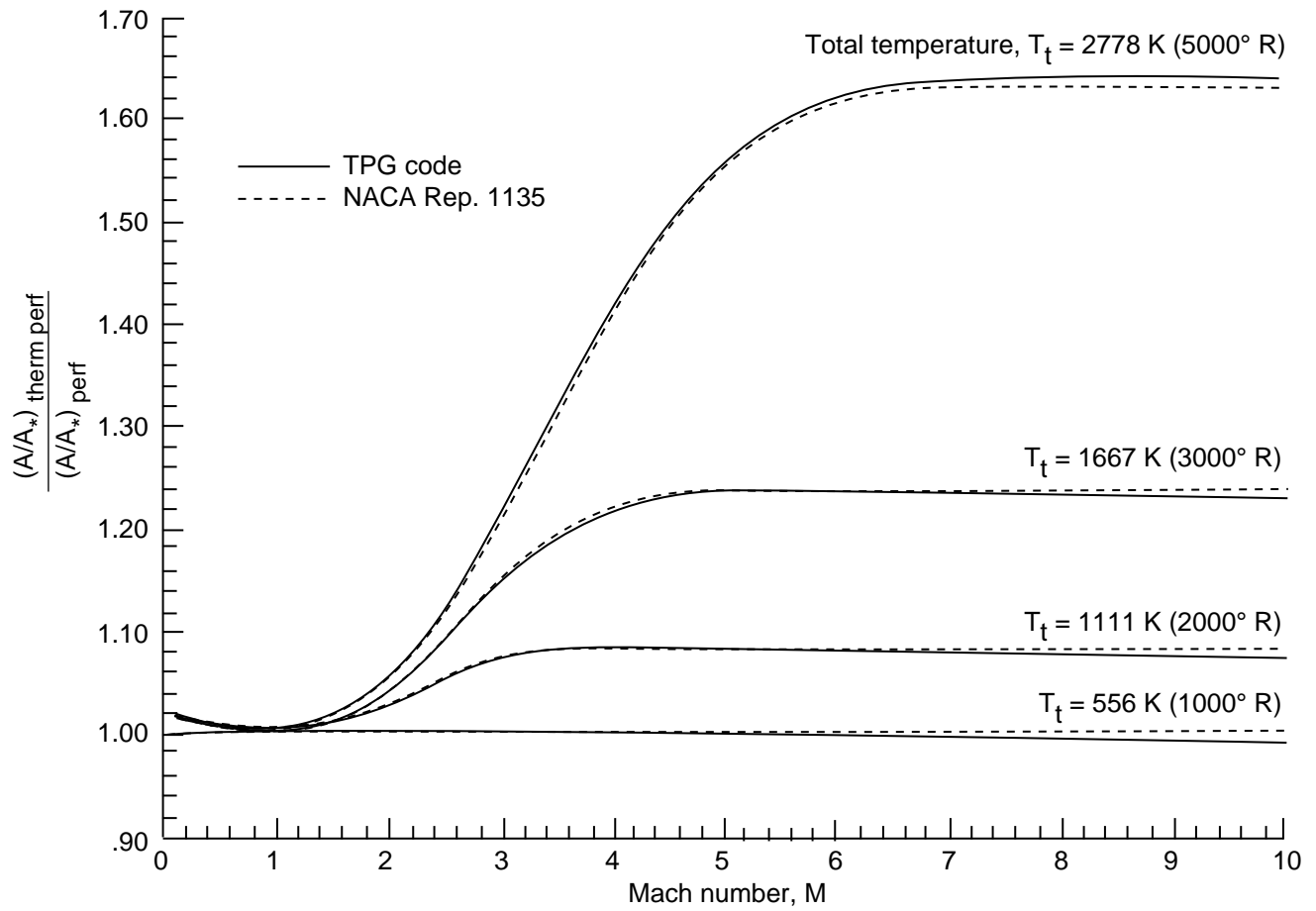


Figure 9. Effect of caloric imperfections on ratio of local cross-sectional area of stream tube to cross-sectional area at $M = 1$.

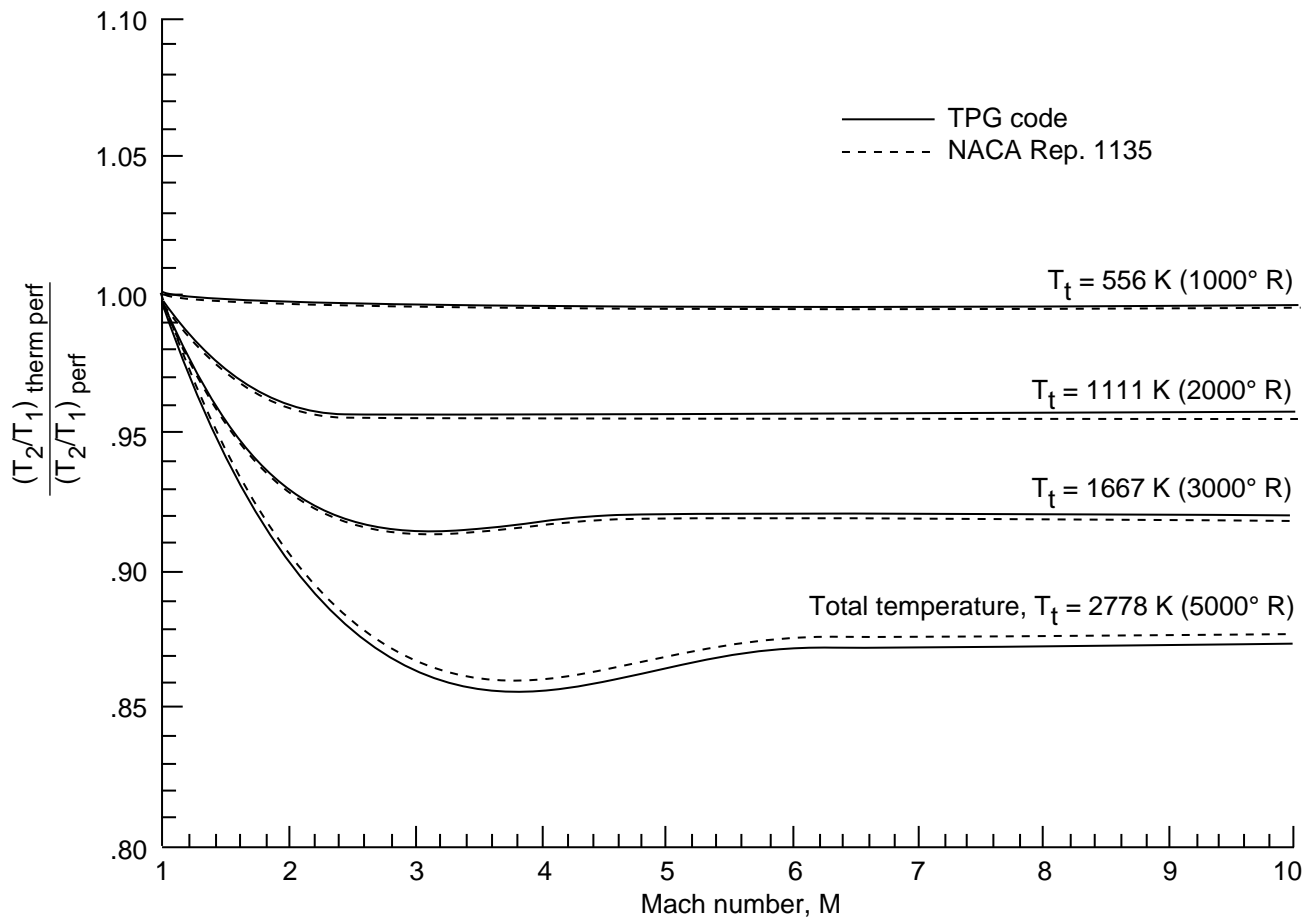


Figure 10. Effect of caloric imperfections on static temperature ratio across normal shock wave.

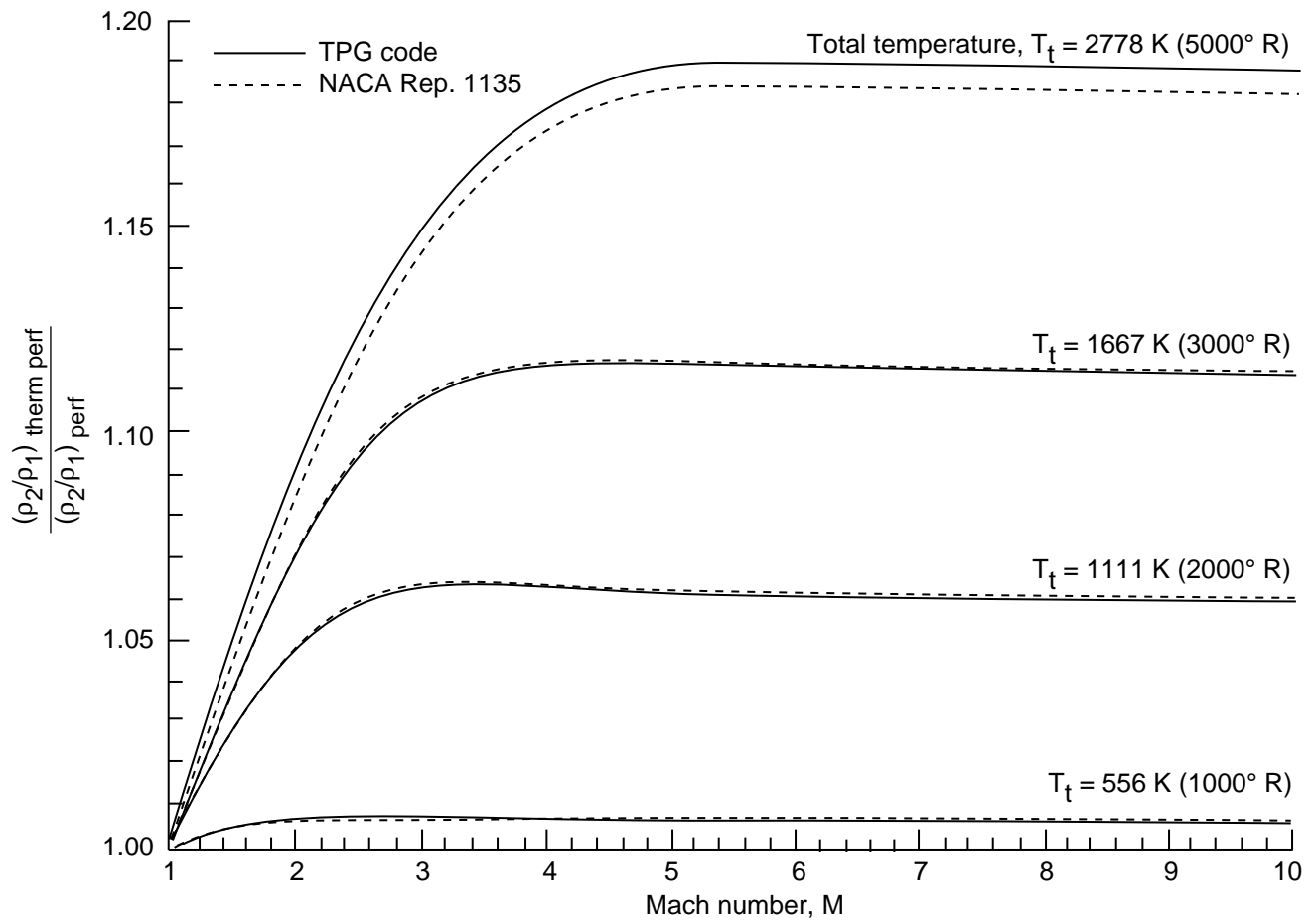


Figure 11. Effect of caloric imperfections on static density ratio across normal shock wave.

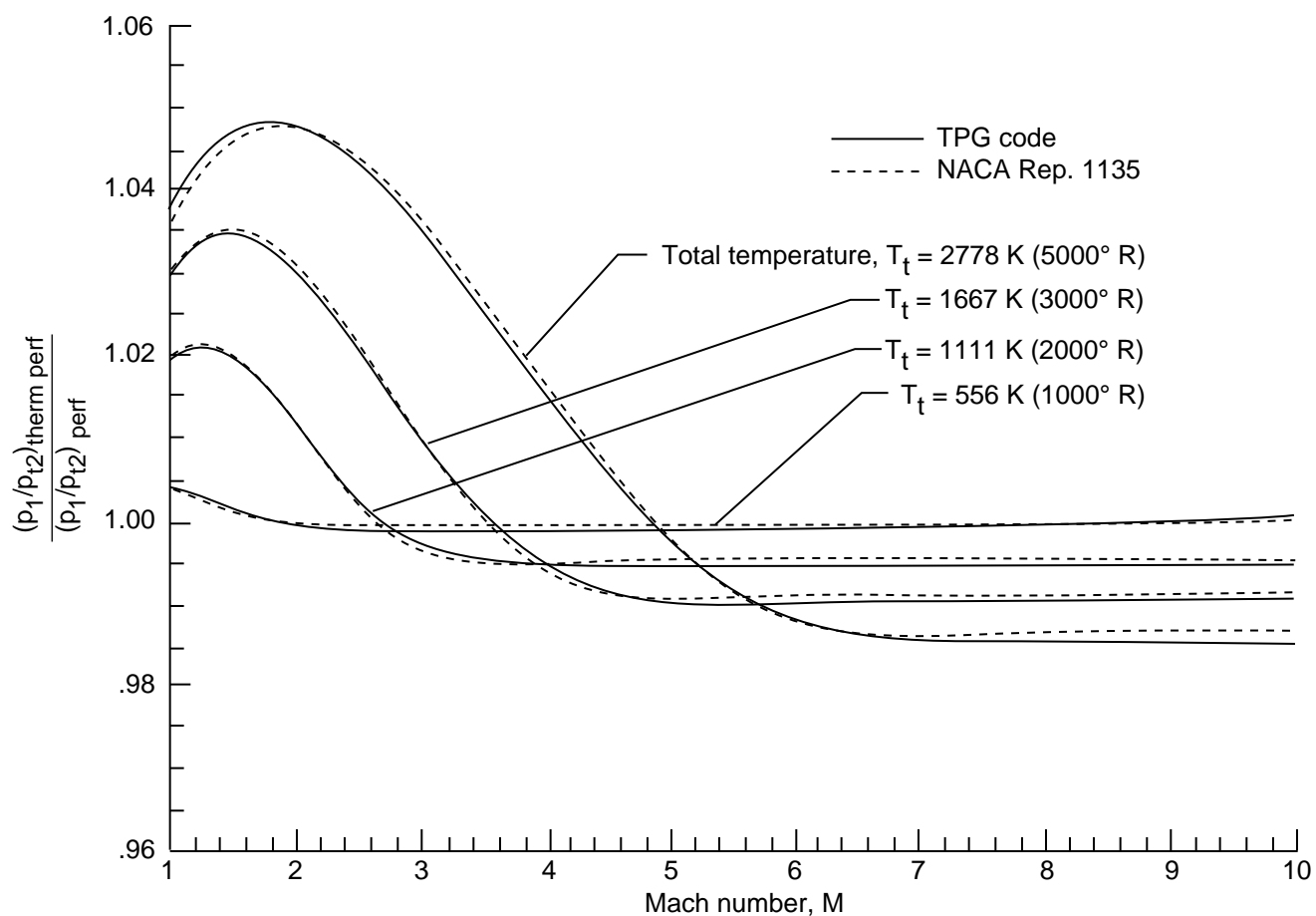


Figure 12. Effect of caloric imperfections on ratio of static pressure upstream of normal shock wave to total pressure downstream.

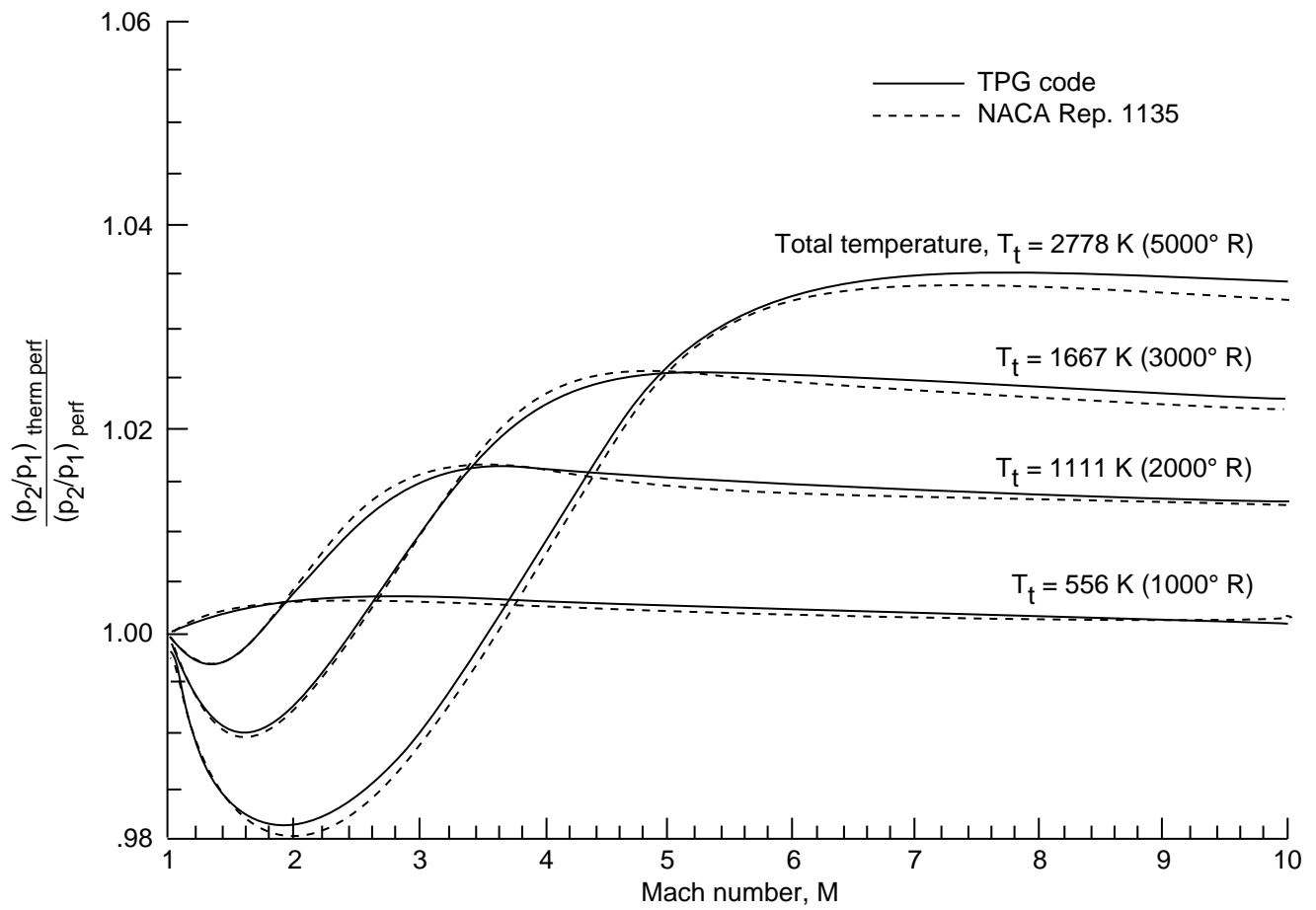


Figure 13. Effect of caloric imperfections on static pressure ratio across normal shock wave.

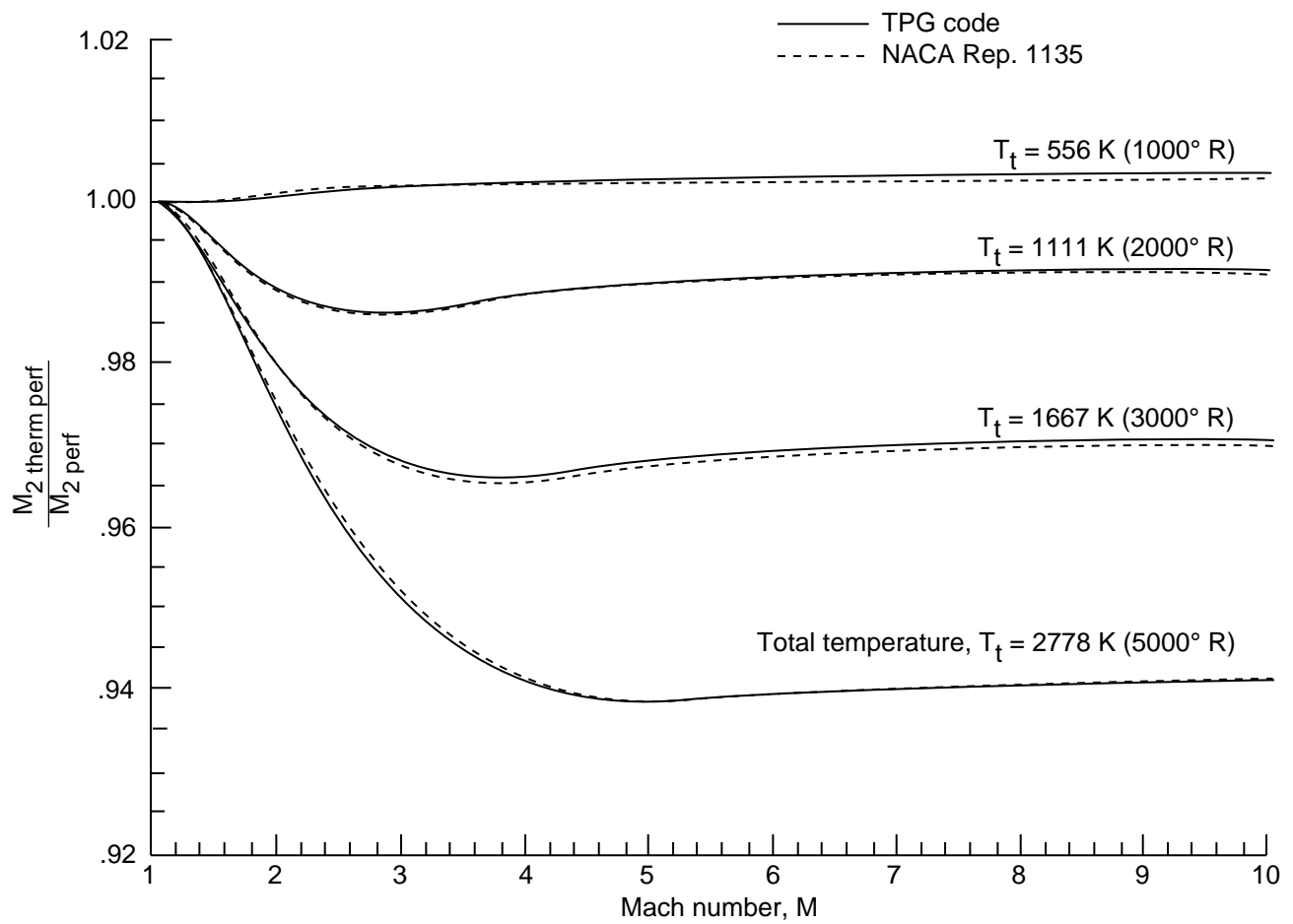


Figure 14. Effect of caloric imperfections on Mach number downstream of normal shock wave.

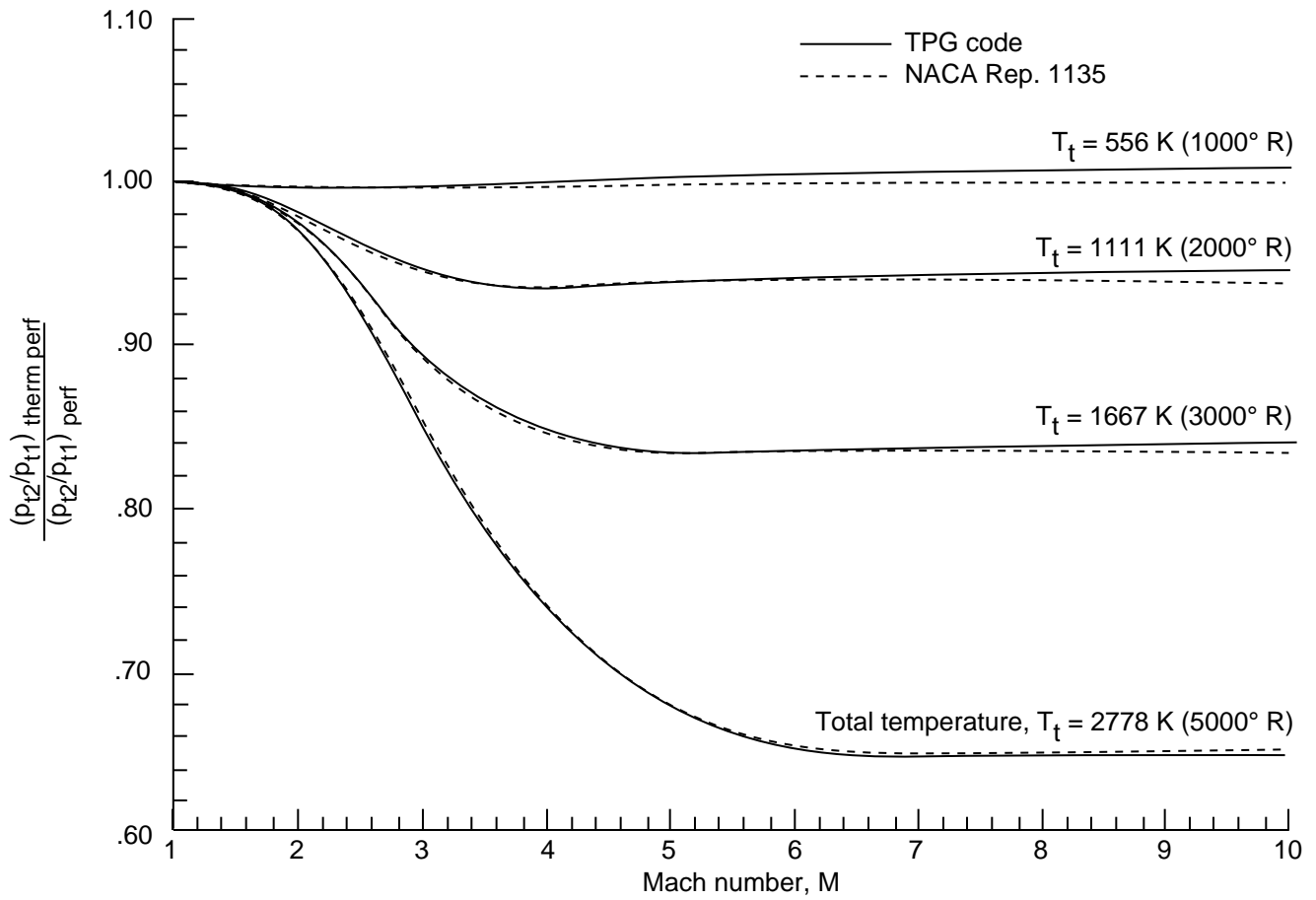


Figure 15. Effect of caloric imperfections on total pressure ratio across normal shock wave.

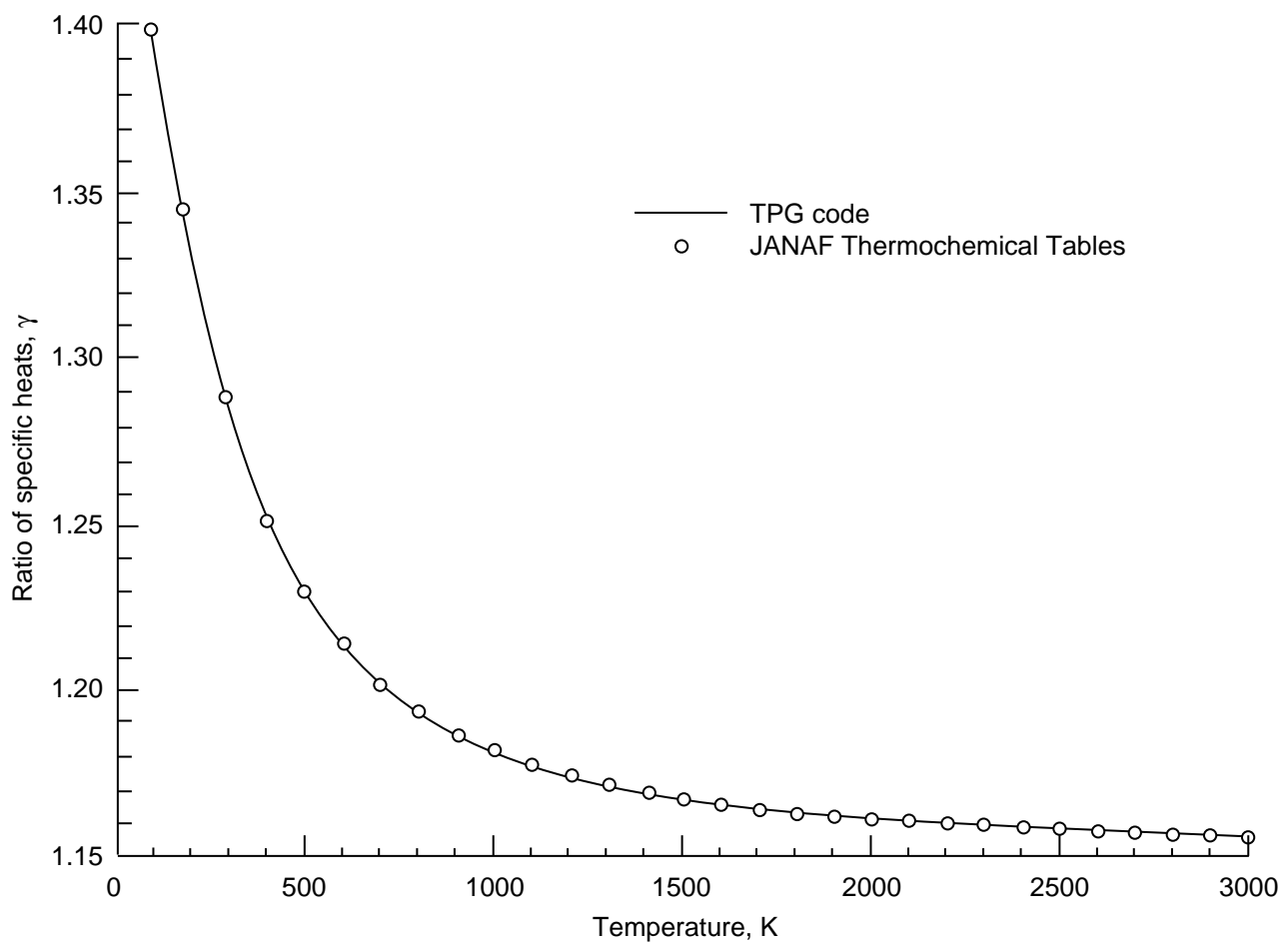


Figure 16. Variation of ratio of specific heats with temperature for thermally perfect CO_2 .

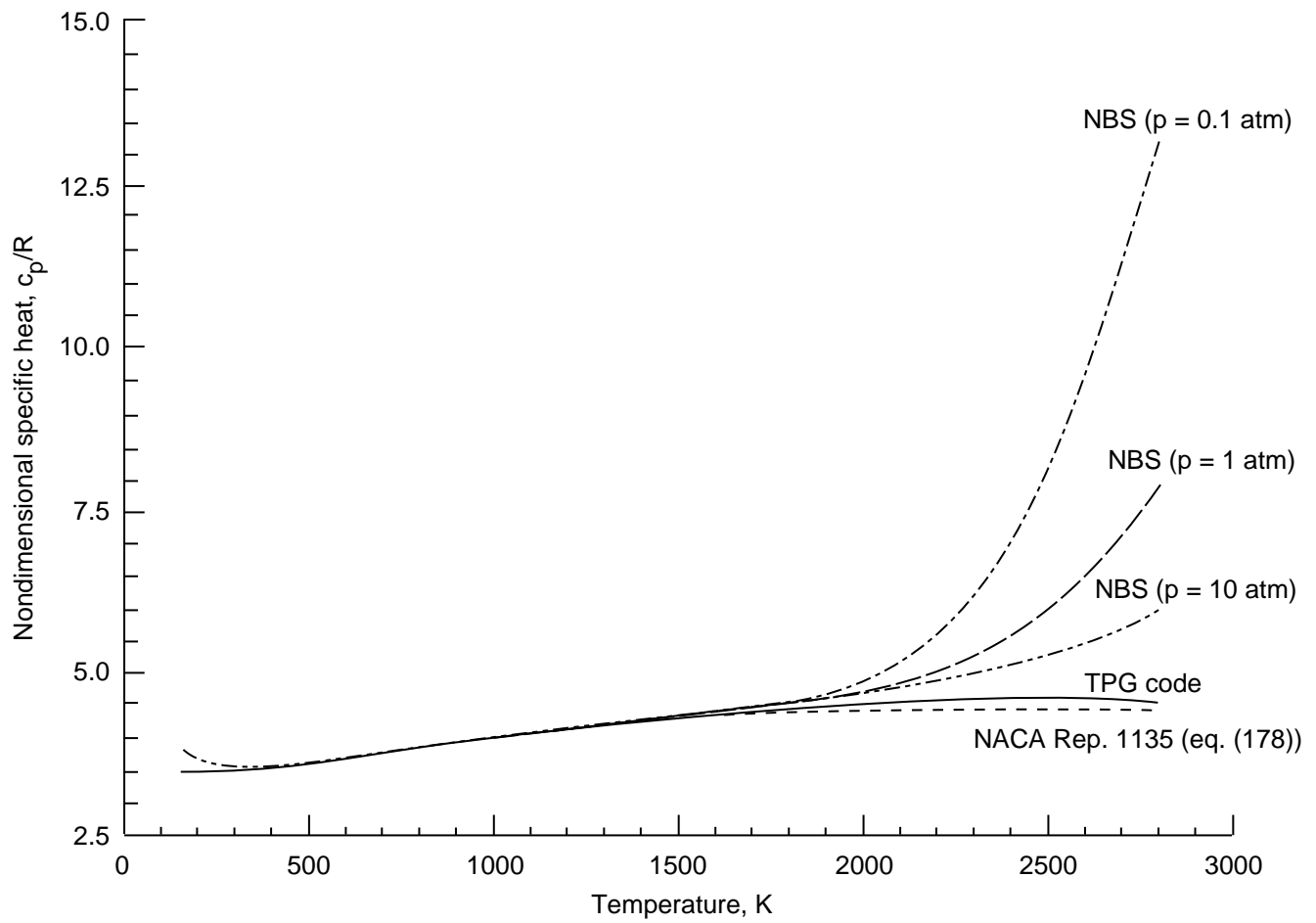


Figure 17. Variation of specific heat (nondimensionalized by gas constant) with temperature for air.

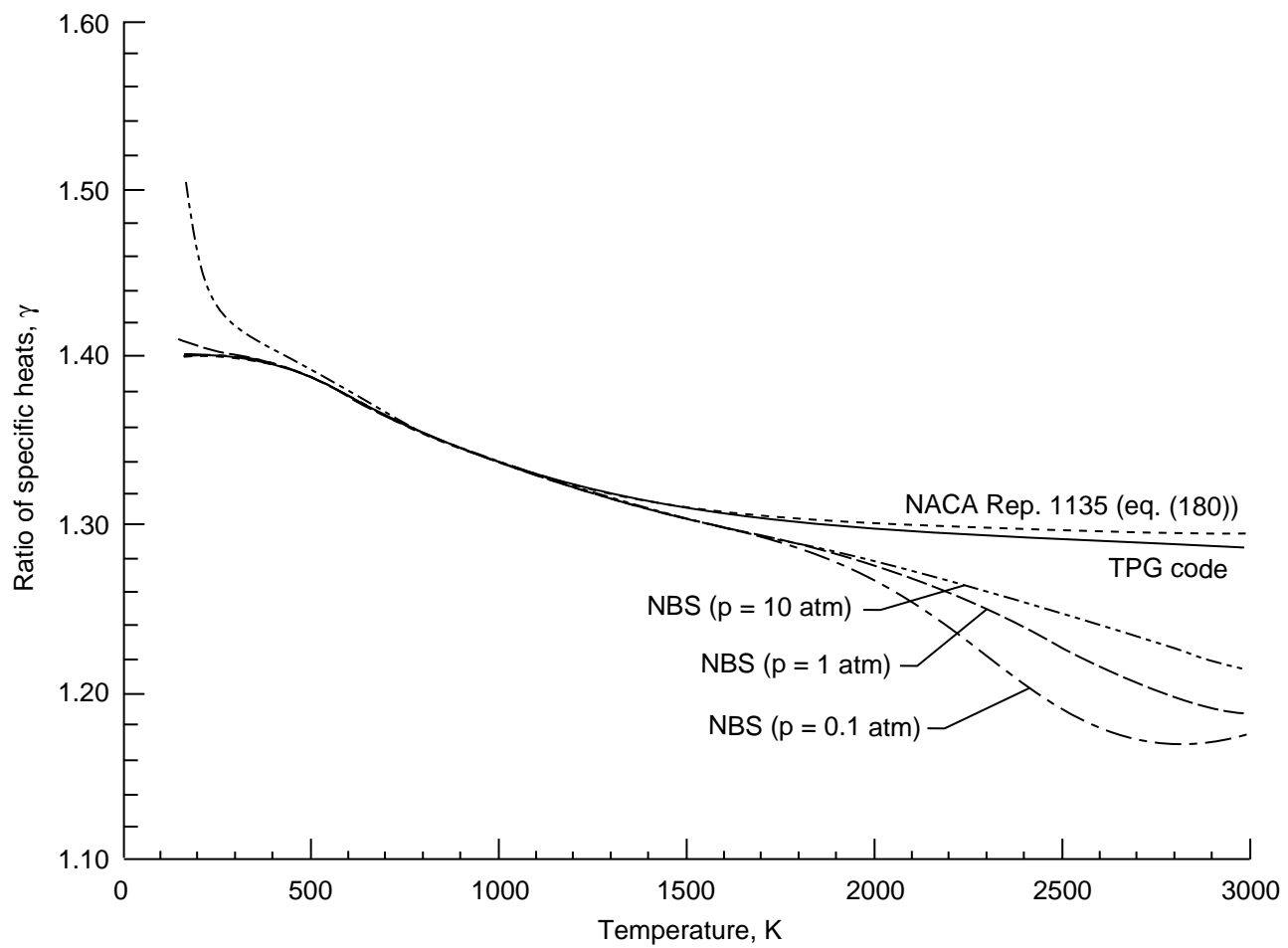


Figure 18. Variation of ratio of specific heats with temperature for air.

Appendix A

This appendix presents a listing of the TPG FORTRAN source code, as released with this report, and described herein. The include files are listed first, containing certain parameter statements, common blocks, and variables specifications which are accessed by multiple routines. The main program, **TPG.f**, is listed next, followed by the other “.f” files, which contain the program subroutines.

Table 5. Database File for Standard Four-Species Composition of Air

Table 6. **TPG.out** File for Calorically Perfect Temperature Regime Test Case

(a) TPG code run in static temperature increment mode

Table 6. Continued

(a) Continued

Table 6(a). Continued

Table 6(a). Concluded

Table 6. Continued

(b) TPG code run in Mach number increment mode

Table 6(b). Continued

Table 6(b). Continued

Table 6(b). Concluded

Table 7. **TPG.out** File for CO₂ Test Case

Table 8. Database File for Steam Sample Case

Table 9. Database File for Mixture of Steam and Air Sample Case

Table 10. Database File for Mixture of Tetrafluoromethane and Argon Sample Case

Table 11. Database File for Nitrogen Sample Case

Table 12. **TPG.out** File for Steam Sample Case

Table 12. Concluded

Table 13. **TPG.out** File for Steam and Air Mixture Sample Case

Table 13. Concluded

Table 14. **TPG.out** File for Tetrafluoromethane and Argon Sample Case

Table 14. Concluded

Table 15. **TPG.out** File for Nitrogen Sample Case

Table 15. Continued

Table 15. Concluded

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13. ABSTRACT (Maximum 200 words) A set of one-dimensional compressible flow relations for a thermally perfect, calorically imperfect gas is derived for the specific heat c_p , expressed as a polynomial function of temperature, and developed into the thermally perfect gas (TPG) computer code. The code produces tables of compressible flow properties similar to those of NACA Rep. 1135. Unlike the tables of NACA Rep. 1135 which are valid only in the calorically perfect temperature regime, the TPG code results are also valid in the thermally perfect, calorically imperfect temperature regime, which considerably extends the range of temperature application. Accuracy of the TPG code in the calorically perfect temperature regime is verified by comparisons with the tables of NACA Rep. 1135. In the thermally perfect, calorically imperfect temperature regime, the TPG code is validated by comparisons with results obtained from the method of NACA Rep. 1135 for calculating the thermally perfect, calorically imperfect compressible flow properties. The temperature limits for application of the TPG code are also examined. The advantage of the TPG code is its applicability to any type of gas (monatomic, diatomic, triatomic, polyatomic) or any specified mixture thereof, whereas the method of NACA Rep. 1135 is restricted to only diatomic gases.				
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